

Supporting Information

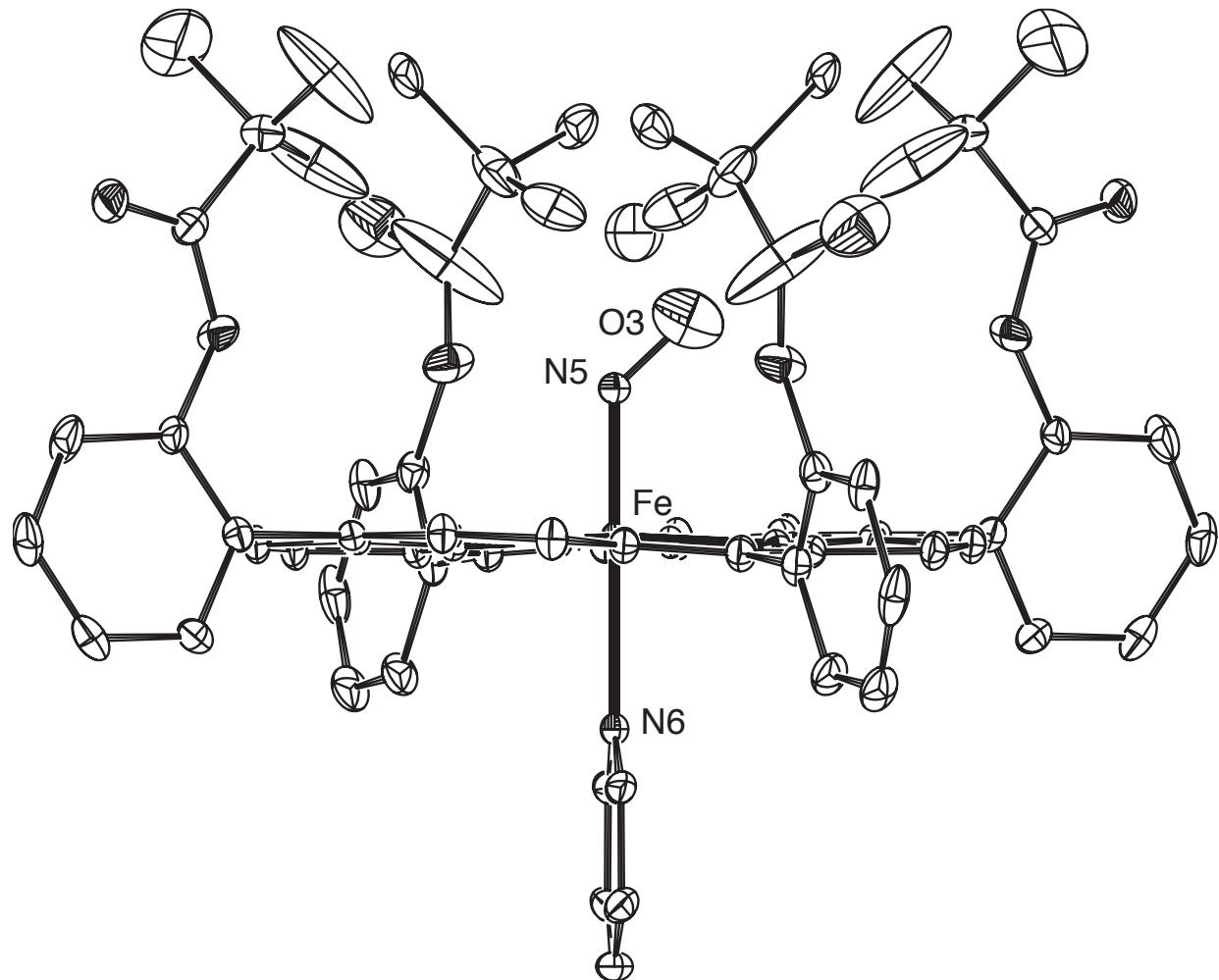
Captions for Supporting Information Figures

Figure S1. ORTEP diagram of [Fe(TpivPP)(NO)(Py)] illustrating 50 % probability ellipsoids.

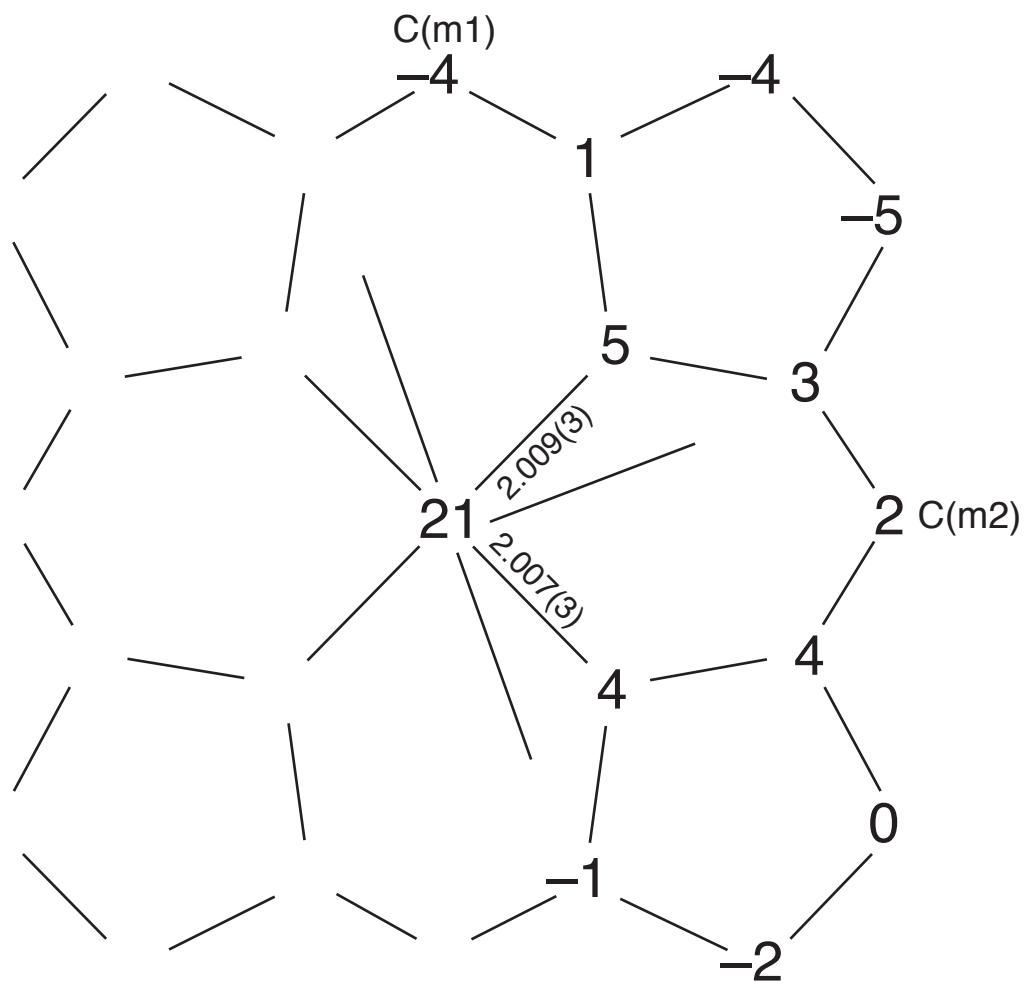
Figure S2. Formal diagram of the porphyrinato core of [Fe(TpivPP)(NO)(Py)] displaying the perpendicular displacements (in units of 0.01 Å) of the core atoms from the 24-atom mean porphyrin plane. Positive displacements are towards the nitrosyl coordinated face of the porphyrin. The projections of the two axial ligands are shown.

Figure S3. Mössbauer spectra of [Fe(TPP)(NO)(4-MePIP)] at 4.2K in an applied field of a) 3 T, b) 6 T, and c) 8.8 T parallel to the γ -ray beam. The solid lines are simultaneous fits to the three spectra without rotation of the EFG tensor. The parameters determined by these fits are listed in Table 5.

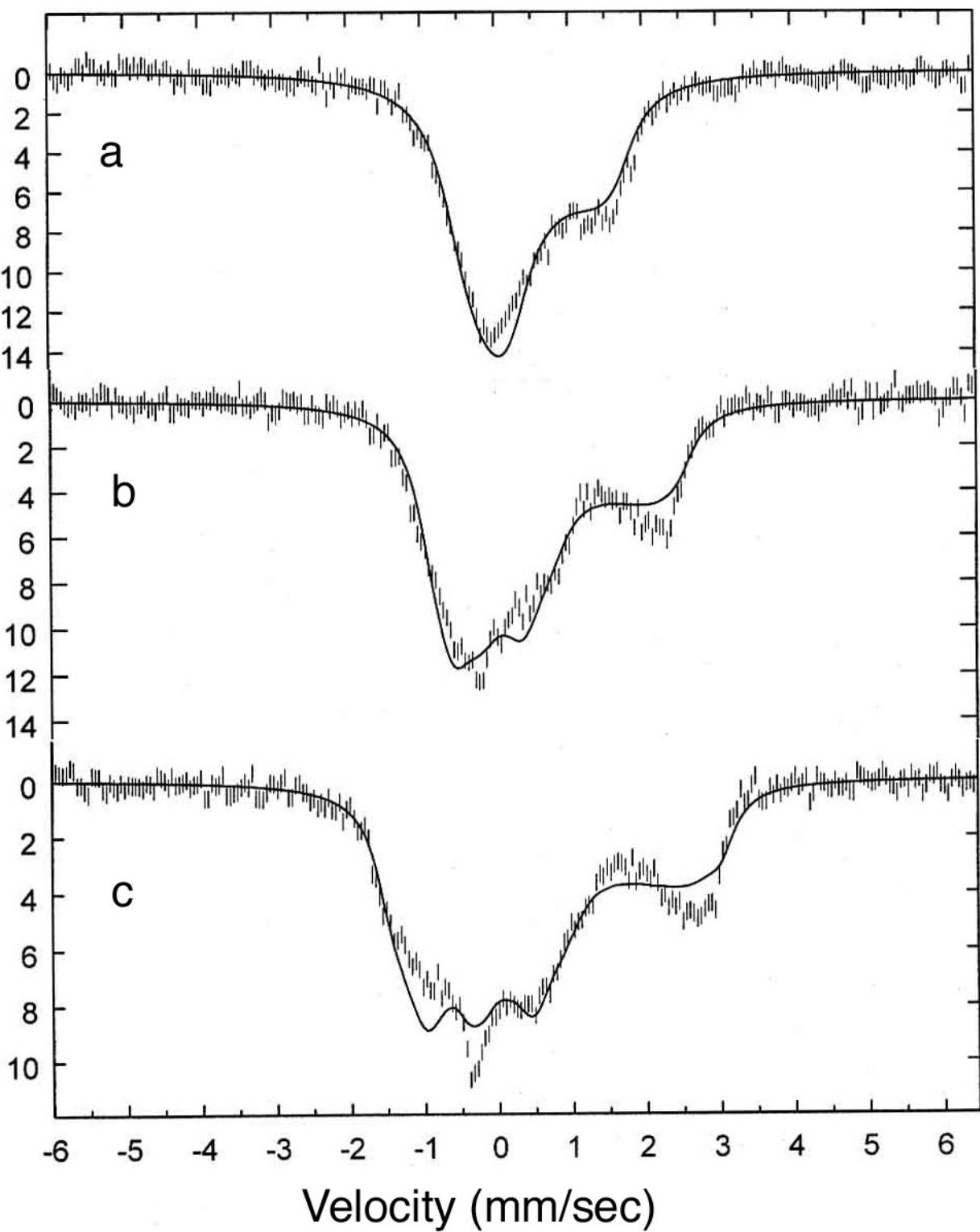
Figure S4. Mössbauer spectra of [Fe(TPP)(NO)(4-MePIP)] at 4.2K in an applied field of a) 3 T, b) 6 T, and c) 8.8 T parallel to the γ -ray beam. The solid lines are simultaneous fits to the three spectra including Euler angles (α) and (β) to model rotation of the EFG tensor. The parameters determined by these fits are listed in Table 5.

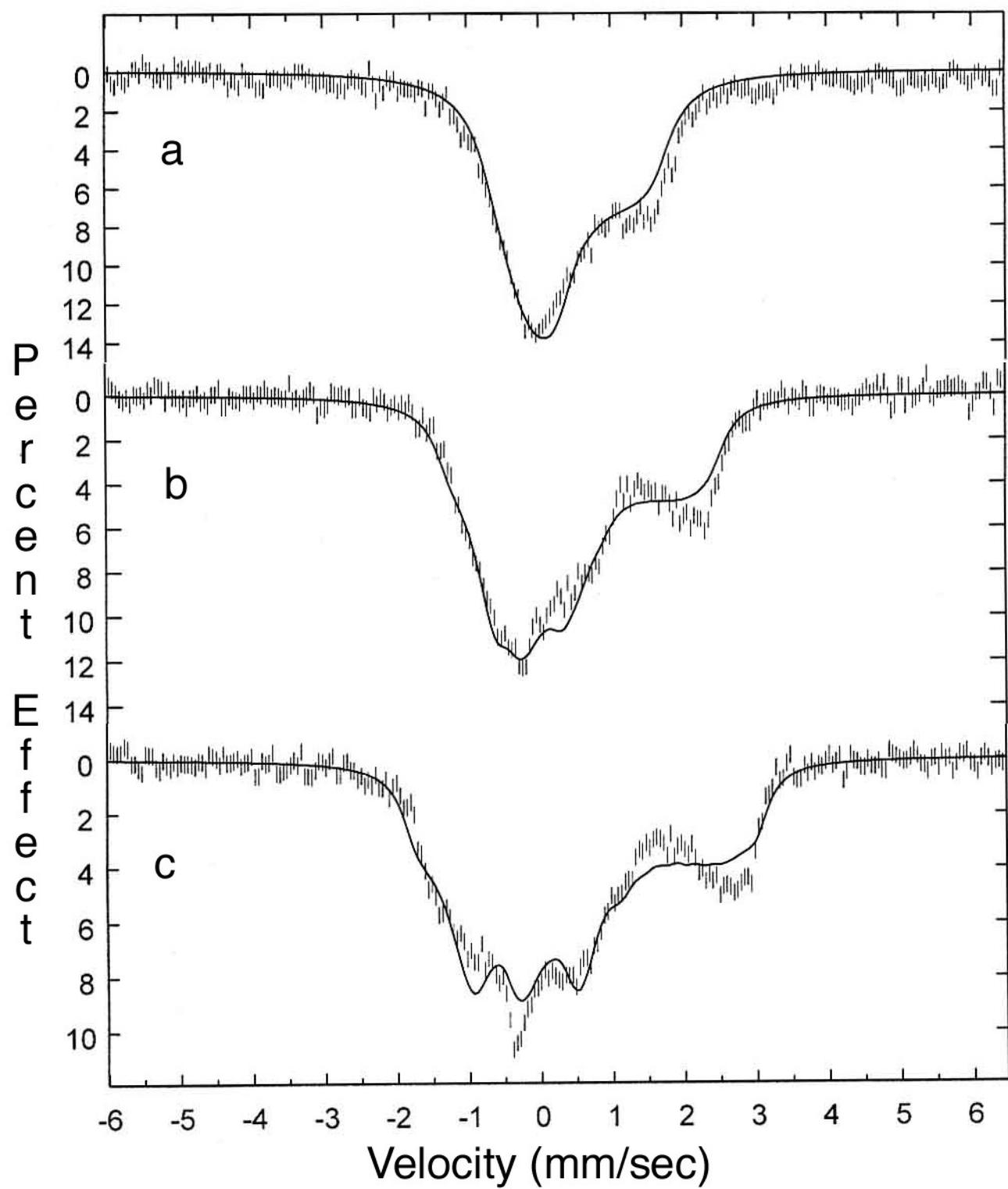


S-2



Percent Effect





Supporting Information

Table S1. Complete Crystallographic Details for [Fe(TPP)(NO)(4-NMe₂Py)]

formula	C ₅₁ H ₃₈ FeN ₇ O
FW, amu	820.73
<i>a</i> , Å	10.8807(7)
<i>b</i> , Å	11.1420(7)
<i>c</i> , Å	17.1221(10)
α , deg	90.1900(10)
β , deg	93.1130(10)
γ , deg	105.6130(10)
<i>V</i> , Å ³	1995.9(2)
space group	<i>P</i> 1̄
<i>Z</i>	2
D _c , g/cm ³	1.366
F(000)	854
μ , mm ⁻¹	0.428
crystal dimensions, mm	0.21 × 0.17 × 0.11
radiation	MoK α , $\bar{\lambda} = 0.71073$ Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.90–30.51
index range	$-15 \leq h \neq 15$ $-15 \leq k \leq 15$ $-24 \leq l \leq 24$
total data collected	25350
absorption correction	Empirical
relative transmission coefficients (I)	1.00000 and 0.920798
unique data	12106 ($R_{\text{int}} = 0.027$)
unique observed data [$I > 2\sigma(I)$]	9401
refinement method	Full-matrix least-squares on F ²
data/restraints/parameters	12106/0/543
goodness-of-fit (based on F^2)	1.031
final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.0464$, $wR_2 = 0.1106$
final <i>R</i> indices (all data)	$R_1 = 0.0632$, $wR_2 = 0.1196$

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(4-NMe₂Py)]^a

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
Fe(1)	0.34951(2)	0.18815(2)	0.21615(1)	0.0148(1)
N(1)	0.20753(12)	0.24094(12)	0.15776(7)	0.0163(2)
N(2)	0.46326(12)	0.36311(12)	0.20879(8)	0.0166(2)
N(3)	0.48636(12)	0.14236(12)	0.28239(7)	0.0159(2)
N(4)	0.23168(12)	0.01889(12)	0.22901(7)	0.0161(2)
N(5)	0.40419(12)	0.13209(12)	0.13235(8)	0.0183(3)
O(1)	0.42843(13)	0.04243(12)	0.10964(8)	0.0298(3)
N(6)	0.27198(13)	0.22979(13)	0.33117(8)	0.0202(3)
C(a1)	0.08560(14)	0.16788(14)	0.13815(9)	0.0170(3)
C(a2)	0.21518(15)	0.35394(14)	0.12335(9)	0.0176(3)
C(a3)	0.43753(14)	0.45884(14)	0.16609(9)	0.0173(3)
C(a4)	0.58857(14)	0.40707(14)	0.23723(9)	0.0167(3)
C(a5)	0.60828(14)	0.21574(14)	0.30162(9)	0.0165(3)
C(a6)	0.47883(14)	0.02953(14)	0.31695(9)	0.0167(3)
C(a7)	0.25989(14)	-0.07915(14)	0.26803(9)	0.0168(3)
C(a8)	0.10747(14)	-0.02581(14)	0.19878(9)	0.0173(3)
C(b1)	0.01462(15)	0.23780(15)	0.09211(9)	0.0204(3)
C(b2)	0.09477(15)	0.35226(15)	0.08231(9)	0.0207(3)
C(b3)	0.54848(15)	0.56522(15)	0.16841(9)	0.0196(3)
C(b4)	0.64177(15)	0.53350(15)	0.21255(9)	0.0202(3)
C(b5)	0.67746(15)	0.14734(15)	0.34996(9)	0.0195(3)
C(b6)	0.59722(15)	0.03278(15)	0.35968(9)	0.0195(3)
C(b7)	0.15117(14)	-0.18744(14)	0.26145(9)	0.0188(3)
C(b8)	0.05764(15)	-0.15444(14)	0.21843(9)	0.0190(3)
C(m1)	0.32222(15)	0.45650(14)	0.12547(9)	0.0173(3)
C(m2)	0.65781(14)	0.33970(14)	0.28071(9)	0.0175(3)
C(m3)	0.37368(14)	-0.07550(14)	0.31061(9)	0.0167(3)
C(m4)	0.03692(14)	0.04352(14)	0.15750(9)	0.0175(3)
C(11)	0.31422(14)	0.56834(14)	0.07930(9)	0.0176(3)
C(12)	0.35808(16)	0.58321(16)	0.00400(10)	0.0231(3)
C(13)	0.35279(16)	0.68777(16)	-0.03888(10)	0.0247(3)
C(14)	0.30459(15)	0.77897(15)	-0.00679(10)	0.0229(3)
C(15)	0.25782(16)	0.76324(16)	0.06733(10)	0.0244(3)
C(16)	0.26209(16)	0.65832(15)	0.10986(10)	0.0222(3)

Table S2. Continued

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
C(21)	0.79397(15)	0.40268(15)	0.30590(9)	0.0196(3)
C(22)	0.82326(18)	0.47496(17)	0.37407(10)	0.0284(4)
C(23)	0.9503(2)	0.52920(19)	0.39918(12)	0.0390(5)
C(24)	1.04794(18)	0.51363(19)	0.35536(14)	0.0402(5)
C(25)	1.01985(18)	0.4457(2)	0.28655(15)	0.0406(5)
C(26)	0.89330(16)	0.38916(17)	0.26162(12)	0.0296(4)
C(31)	0.38342(14)	-0.19002(14)	0.35333(9)	0.0176(3)
C(32)	0.36462(16)	-0.19855(15)	0.43328(9)	0.0217(3)
C(33)	0.37025(17)	-0.30527(16)	0.47321(10)	0.0247(3)
C(34)	0.39507(16)	-0.40475(16)	0.43432(10)	0.0232(3)
C(35)	0.41578(18)	-0.39669(16)	0.35501(11)	0.0269(4)
C(36)	0.41033(17)	-0.28935(16)	0.31497(10)	0.0245(3)
C(41)	-0.10076(14)	-0.01779(14)	0.13471(9)	0.0174(3)
C(42)	-0.13611(16)	-0.09559(16)	0.06906(10)	0.0243(3)
C(43)	-0.26504(17)	-0.14795(17)	0.04742(11)	0.0276(4)
C(44)	-0.35850(16)	-0.12285(16)	0.09119(10)	0.0249(3)
C(45)	-0.32426(16)	-0.04766(17)	0.15767(11)	0.0263(4)
C(46)	-0.19570(15)	0.00512(16)	0.17919(10)	0.0229(3)
C(1)	0.33794(16)	0.24024(16)	0.40056(10)	0.0237(3)
C(2)	0.28511(17)	0.22721(18)	0.47283(10)	0.0273(4)
C(3)	0.15116(17)	0.20013(16)	0.47633(10)	0.0253(3)
C(4)	0.08209(17)	0.19444(17)	0.40413(10)	0.0271(4)
C(5)	0.14478(16)	0.20872(17)	0.33568(10)	0.0249(3)
N(7)	0.09163(16)	0.17975(18)	0.54494(9)	0.0352(4)
C(6)	-0.0477(2)	0.1434(2)	0.54399(13)	0.0394(5)
C(7)	0.1644(2)	0.1830(3)	0.61914(12)	0.0490(6)

^a *U*(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S3. Bond Lengths for [Fe(TPP)(NO)(4-NMe₂Py)]^a

bond	length (Å)	bond	length (Å)
Fe(1)–N(5)	1.7577(13)	C(m1)–C(11)	1.498(2)
Fe(1)–N(4)	1.9952(13)	C(m2)–C(21)	1.497(2)
Fe(1)–N(3)	1.9982(13)	C(m3)–C(31)	1.498(2)
Fe(1)–N(1)	2.0143(13)	C(m4)–C(41)	1.499(2)
Fe(1)–N(2)	2.0169(13)	C(11)–C(16)	1.391(2)
Fe(1)–N(6)	2.2783(13)	C(11)–C(12)	1.394(2)
N(1)–C(a2)	1.3759(19)	C(12)–C(13)	1.392(2)
N(1)–C(a1)	1.3798(19)	C(13)–C(14)	1.387(2)
N(2)–C(a3)	1.3763(19)	C(14)–C(15)	1.387(2)
N(2)–C(a4)	1.3794(19)	C(15)–C(16)	1.389(2)
N(3)–C(a6)	1.3755(19)	C(21)–C(22)	1.388(2)
N(3)–C(a5)	1.3797(18)	C(21)–C(26)	1.393(2)
N(4)–C(a7)	1.3773(19)	C(22)–C(23)	1.395(3)
N(4)–C(a8)	1.3793(19)	C(23)–C(24)	1.381(3)
N(5)–O(1)	1.1700(17)	C(24)–C(25)	1.373(3)
N(6)–C(1)	1.342(2)	C(25)–C(26)	1.394(3)
N(6)–C(5)	1.347(2)	C(31)–C(36)	1.390(2)
C(a1)–C(m4)	1.392(2)	C(31)–C(32)	1.395(2)
C(a1)–C(b1)	1.444(2)	C(32)–C(33)	1.388(2)
C(a2)–C(m1)	1.394(2)	C(33)–C(34)	1.386(2)
C(a2)–C(b2)	1.448(2)	C(34)–C(35)	1.388(2)
C(a3)–C(m1)	1.395(2)	C(35)–C(36)	1.394(2)
C(a3)–C(b3)	1.445(2)	C(41)–C(42)	1.389(2)
C(a4)–C(m2)	1.390(2)	C(41)–C(46)	1.392(2)
C(a4)–C(b4)	1.446(2)	C(42)–C(43)	1.395(2)
C(a5)–C(m2)	1.396(2)	C(43)–C(44)	1.382(3)
C(a5)–C(b5)	1.441(2)	C(44)–C(45)	1.384(3)
C(a6)–C(m3)	1.398(2)	C(45)–C(46)	1.392(2)
C(a6)–C(b6)	1.438(2)	C(1)–C(2)	1.384(2)
C(a7)–C(m3)	1.393(2)	C(2)–C(3)	1.411(2)
C(a7)–C(b7)	1.444(2)	C(3)–N(7)	1.363(2)
C(a8)–C(m4)	1.396(2)	C(3)–C(4)	1.403(3)
C(a8)–C(b8)	1.437(2)	C(4)–C(5)	1.376(2)
C(b1)–C(b2)	1.354(2)	N(7)–C(7)	1.455(3)

Table S3. Continued

bond	length (Å)	bond	length (Å)
C(b3)–C(b4)	1.356(2)	N(7)–C(6)	1.459(3)
C(b5)–C(b6)	1.355(2)		
C(b7)–C(b8)	1.355(2)		

^aThe estimated standard deviations of the least significant digits are given in parentheses.

Table S4. Bond Angles for [Fe(TPP)(NO)(4-NMe₂Py)]^a

angle	degree	angle	degree
N(5)–Fe(1)–N(4)	88.85(6)	C(b6)–C(b5)–C(a5)	106.94(14)
N(5)–Fe(1)–N(3)	90.19(6)	C(b5)–C(b6)–C(a6)	107.07(14)
N(4)–Fe(1)–N(3)	90.70(5)	C(b8)–C(b7)–C(a7)	107.05(14)
N(5)–Fe(1)–N(1)	94.75(6)	C(b7)–C(b8)–C(a8)	106.99(13)
N(4)–Fe(1)–N(1)	89.82(5)	C(a2)–C(m1)–C(a3)	123.50(14)
N(3)–Fe(1)–N(1)	175.05(5)	C(a2)–C(m1)–C(11)	118.10(14)
N(5)–Fe(1)–N(2)	94.77(6)	C(a3)–C(m1)–C(11)	118.36(13)
N(4)–Fe(1)–N(2)	176.35(5)	C(a4)–C(m2)–C(a5)	123.80(14)
N(3)–Fe(1)–N(2)	89.71(5)	C(a4)–C(m2)–C(21)	118.38(14)
N(1)–Fe(1)–N(2)	89.46(5)	C(a5)–C(m2)–C(21)	117.81(14)
N(5)–Fe(1)–N(6)	171.12(6)	C(a7)–C(m3)–C(a6)	123.86(14)
N(4)–Fe(1)–N(6)	83.29(5)	C(a7)–C(m3)–C(31)	118.20(13)
N(3)–Fe(1)–N(6)	85.80(5)	C(a6)–C(m3)–C(31)	117.94(13)
N(1)–Fe(1)–N(6)	89.37(5)	C(a1)–C(m4)–C(a8)	123.93(14)
N(2)–Fe(1)–N(6)	93.12(5)	C(a1)–C(m4)–C(41)	117.69(13)
C(a2)–N(1)–C(a1)	105.61(12)	C(a8)–C(m4)–C(41)	118.35(14)
C(a2)–N(1)–Fe(1)	127.10(10)	C(16)–C(11)–C(12)	118.73(15)
C(a1)–N(1)–Fe(1)	127.08(10)	C(16)–C(11)–C(m1)	121.13(14)
C(a3)–N(2)–C(a4)	105.55(12)	C(12)–C(11)–C(m1)	120.13(14)
C(a3)–N(2)–Fe(1)	126.96(10)	C(13)–C(12)–C(11)	120.53(15)
C(a4)–N(2)–Fe(1)	127.04(10)	C(14)–C(13)–C(12)	120.23(16)
C(a6)–N(3)–C(a5)	105.78(12)	C(13)–C(14)–C(15)	119.52(15)
C(a6)–N(3)–Fe(1)	126.78(10)	C(14)–C(15)–C(16)	120.21(16)
C(a5)–N(3)–Fe(1)	127.42(10)	C(15)–C(16)–C(11)	120.72(15)
C(a7)–N(4)–C(a8)	105.76(12)	C(22)–C(21)–C(26)	118.93(16)
C(a7)–N(4)–Fe(1)	126.65(10)	C(22)–C(21)–C(m2)	120.47(15)
C(a8)–N(4)–Fe(1)	127.55(10)	C(26)–C(21)–C(m2)	120.60(15)
O(1)–N(5)–Fe(1)	139.79(12)	C(21)–C(22)–C(23)	120.38(18)
C(1)–N(6)–C(5)	114.62(14)	C(24)–C(23)–C(22)	120.11(19)
C(1)–N(6)–Fe(1)	123.77(11)	C(25)–C(24)–C(23)	119.93(18)
C(5)–N(6)–Fe(1)	118.91(11)	C(24)–C(25)–C(26)	120.4(2)
N(1)–C(a1)–C(m4)	125.75(14)	C(21)–C(26)–C(25)	120.17(19)
N(1)–C(a1)–C(b1)	110.32(13)	C(36)–C(31)–C(32)	118.71(15)
C(m4)–C(a1)–C(b1)	123.91(14)	C(36)–C(31)–C(m3)	121.46(14)

Table S4. Continued

angle	degree	angle	degree
N(1)–C(a2)–C(m1)	126.23(14)	C(32)–C(31)–C(m3)	119.83(14)
N(1)–C(a2)–C(b2)	110.25(13)	C(33)–C(32)–C(31)	120.47(15)
C(m1)–C(a2)–C(b2)	123.51(14)	C(34)–C(33)–C(32)	120.50(16)
N(2)–C(a3)–C(m1)	126.14(14)	C(33)–C(34)–C(35)	119.58(16)
N(2)–C(a3)–C(b3)	110.34(13)	C(34)–C(35)–C(36)	119.87(16)
C(m1)–C(a3)–C(b3)	123.53(14)	C(31)–C(36)–C(35)	120.86(16)
N(2)–C(a4)–C(m2)	125.86(14)	C(42)–C(41)–C(46)	119.03(15)
N(2)–C(a4)–C(b4)	110.38(13)	C(42)–C(41)–C(m4)	121.36(14)
C(m2)–C(a4)–C(b4)	123.71(14)	C(46)–C(41)–C(m4)	119.60(14)
N(3)–C(a5)–C(m2)	125.91(14)	C(41)–C(42)–C(43)	120.28(16)
N(3)–C(a5)–C(b5)	109.99(13)	C(44)–C(43)–C(42)	120.22(16)
C(m2)–C(a5)–C(b5)	124.05(14)	C(43)–C(44)–C(45)	119.93(16)
N(3)–C(a6)–C(m3)	125.83(14)	C(44)–C(45)–C(46)	119.95(16)
N(3)–C(a6)–C(b6)	110.21(13)	C(45)–C(46)–C(41)	120.56(16)
C(m3)–C(a6)–C(b6)	123.94(14)	N(6)–C(1)–C(2)	125.37(16)
N(4)–C(a7)–C(m3)	126.04(14)	C(1)–C(2)–C(3)	119.20(16)
N(4)–C(a7)–C(b7)	109.95(13)	N(7)–C(3)–C(4)	121.68(16)
C(m3)–C(a7)–C(b7)	123.96(14)	N(7)–C(3)–C(2)	122.65(17)
N(4)–C(a8)–C(m4)	125.69(14)	C(4)–C(3)–C(2)	115.67(16)
N(4)–C(a8)–C(b8)	110.24(13)	C(5)–C(4)–C(3)	120.09(16)
C(m4)–C(a8)–C(b8)	124.03(14)	N(6)–C(5)–C(4)	124.95(16)
C(b2)–C(b1)–C(a1)	106.90(14)	C(3)–N(7)–C(7)	121.00(17)
C(b1)–C(b2)–C(a2)	106.90(14)	C(3)–N(7)–C(6)	119.84(17)
C(b4)–C(b3)–C(a3)	107.00(14)	C(7)–N(7)–C(6)	118.95(16)
C(b3)–C(b4)–C(a4)	106.73(14)		

^aThe estimated standard deviations of the least significant digits are given in parentheses.

Table S5. Anisotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(4-NMe₂Py)]^a

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0123(1)	0.0139(1)	0.0176(1)	0.0019(1)	0.0013(1)	0.0026(1)
N(1)	0.0140(6)	0.0154(6)	0.0190(6)	0.0012(5)	0.0017(5)	0.0031(5)
N(2)	0.0148(6)	0.0150(6)	0.0199(6)	0.0017(5)	0.0015(5)	0.0036(5)
N(3)	0.0129(6)	0.0155(6)	0.0188(6)	0.0012(5)	0.0016(5)	0.0025(5)
N(4)	0.0139(6)	0.0167(6)	0.0180(6)	0.0023(5)	0.0025(5)	0.0041(5)
N(5)	0.0147(6)	0.0193(6)	0.0202(6)	0.0018(5)	0.0016(5)	0.0030(5)
O(1)	0.0350(7)	0.0244(6)	0.0323(7)	-0.0022(5)	0.0101(6)	0.0105(5)
N(6)	0.0192(6)	0.0199(6)	0.0215(6)	0.0002(5)	0.0029(5)	0.0050(5)
C(A1)	0.0141(6)	0.0183(7)	0.0187(7)	0.0008(5)	0.0012(5)	0.0043(5)
C(A2)	0.0173(7)	0.0176(7)	0.0187(7)	0.0017(5)	0.0004(5)	0.0061(6)
C(A3)	0.0169(7)	0.0156(7)	0.0191(7)	0.0013(5)	0.0036(5)	0.0032(5)
C(A4)	0.0149(7)	0.0156(7)	0.0183(7)	0.0007(5)	0.0019(5)	0.0019(5)
C(A5)	0.0127(6)	0.0194(7)	0.0174(7)	-0.0004(5)	0.0007(5)	0.0046(5)
C(A6)	0.0165(7)	0.0173(7)	0.0174(7)	0.0015(5)	0.0015(5)	0.0062(5)
C(A7)	0.0165(7)	0.0161(7)	0.0178(7)	0.0032(5)	0.0048(5)	0.0038(5)
C(A8)	0.0152(7)	0.0170(7)	0.0187(7)	0.0015(5)	0.0037(5)	0.0022(5)
C(B1)	0.0162(7)	0.0217(7)	0.0237(8)	0.0024(6)	-0.0020(6)	0.0062(6)
C(B2)	0.0192(7)	0.0202(7)	0.0234(8)	0.0039(6)	-0.0012(6)	0.0070(6)
C(B3)	0.0187(7)	0.0154(7)	0.0232(8)	0.0034(6)	0.0019(6)	0.0022(6)
C(B4)	0.0174(7)	0.0164(7)	0.0249(8)	0.0029(6)	0.0024(6)	0.0012(6)
C(B5)	0.0164(7)	0.0209(7)	0.0211(7)	0.0024(6)	-0.0004(6)	0.0053(6)
C(B6)	0.0169(7)	0.0189(7)	0.0229(7)	0.0031(6)	-0.0002(6)	0.0055(6)
C(B7)	0.0168(7)	0.0166(7)	0.0219(7)	0.0032(6)	0.0033(6)	0.0021(6)
C(B8)	0.0151(7)	0.0184(7)	0.0215(7)	0.0015(6)	0.0028(6)	0.0006(6)
C(M1)	0.0190(7)	0.0166(7)	0.0172(7)	0.0020(5)	0.0031(5)	0.0057(6)
C(M2)	0.0145(7)	0.0184(7)	0.0191(7)	0.0001(6)	0.0020(5)	0.0030(6)
C(M3)	0.0168(7)	0.0174(7)	0.0167(7)	0.0015(5)	0.0028(5)	0.0054(5)
C(M4)	0.0131(6)	0.0199(7)	0.0187(7)	-0.0001(6)	0.0016(5)	0.0030(5)
C(11)	0.0152(7)	0.0164(7)	0.0205(7)	0.0025(5)	0.0008(5)	0.0033(5)
C(12)	0.0233(8)	0.0221(8)	0.0247(8)	0.0026(6)	0.0058(6)	0.0064(6)
C(13)	0.0239(8)	0.0269(8)	0.0221(8)	0.0068(6)	0.0050(6)	0.0038(7)
C(14)	0.0182(7)	0.0200(8)	0.0285(8)	0.0069(6)	-0.0019(6)	0.0019(6)
C(15)	0.0253(8)	0.0187(8)	0.0309(9)	0.0033(6)	0.0029(7)	0.0085(6)
C(16)	0.0251(8)	0.0202(8)	0.0224(8)	0.0025(6)	0.0054(6)	0.0071(6)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(21)	0.0158(7)	0.0176(7)	0.0233(8)	0.0050(6)	0.0003(6)	0.0012(6)
C(22)	0.0254(8)	0.0280(9)	0.0256(8)	0.0029(7)	-0.0016(7)	-0.0029(7)
C(23)	0.0393(11)	0.0293(10)	0.0359(10)	0.0083(8)	-0.0167(9)	-0.0086(8)
C(24)	0.0211(9)	0.0282(10)	0.0620(14)	0.0187(9)	-0.0134(9)	-0.0066(7)
C(25)	0.0163(8)	0.0339(11)	0.0700(15)	0.0115(10)	0.0052(9)	0.0031(7)
C(26)	0.0184(8)	0.0290(9)	0.0400(10)	-0.0003(8)	0.0047(7)	0.0035(7)
C(31)	0.0154(7)	0.0164(7)	0.0207(7)	0.0024(5)	0.0008(5)	0.0037(5)
C(32)	0.0225(8)	0.0201(8)	0.0223(8)	0.0010(6)	0.0029(6)	0.0052(6)
C(33)	0.0275(8)	0.0242(8)	0.0212(8)	0.0053(6)	0.0021(6)	0.0045(7)
C(34)	0.0207(7)	0.0205(8)	0.0277(8)	0.0071(6)	-0.0011(6)	0.0047(6)
C(35)	0.0321(9)	0.0216(8)	0.0304(9)	0.0023(7)	0.0036(7)	0.0128(7)
C(36)	0.0318(9)	0.0235(8)	0.0215(8)	0.0036(6)	0.0048(7)	0.0124(7)
C(41)	0.0147(7)	0.0163(7)	0.0204(7)	0.0031(5)	0.0002(5)	0.0030(5)
C(42)	0.0211(8)	0.0276(8)	0.0232(8)	-0.0025(6)	0.0009(6)	0.0052(6)
C(43)	0.0257(8)	0.0251(9)	0.0278(9)	-0.0023(7)	-0.0069(7)	0.0011(7)
C(44)	0.0168(7)	0.0215(8)	0.0324(9)	0.0070(7)	-0.0044(6)	-0.0005(6)
C(45)	0.0164(7)	0.0308(9)	0.0314(9)	0.0054(7)	0.0043(6)	0.0050(7)
C(46)	0.0175(7)	0.0265(8)	0.0237(8)	-0.0019(6)	0.0003(6)	0.0046(6)
C(1)	0.0189(7)	0.0279(8)	0.0242(8)	-0.0024(6)	0.0017(6)	0.0059(6)
C(2)	0.0262(8)	0.0348(10)	0.0227(8)	-0.0008(7)	0.0008(7)	0.0113(7)
C(3)	0.0278(8)	0.0258(8)	0.0246(8)	-0.0005(6)	0.0076(7)	0.0103(7)
C(4)	0.0202(8)	0.0334(9)	0.0283(9)	-0.0013(7)	0.0052(7)	0.0073(7)
C(5)	0.0203(8)	0.0308(9)	0.0238(8)	-0.0014(7)	0.0008(6)	0.0075(7)
N(7)	0.0328(8)	0.0523(11)	0.0251(8)	0.0044(7)	0.0120(7)	0.0171(8)
C(6)	0.0368(11)	0.0429(12)	0.0395(11)	0.0024(9)	0.0189(9)	0.0094(9)
C(7)	0.0538(14)	0.0842(19)	0.0249(10)	0.0132(11)	0.0138(9)	0.0436(14)

^aThe estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2 \pi [h^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Table S6. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(4-NMe₂Py)]^a

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
H(B1)	-0.0718	0.2090	0.0725	0.024
H(B2)	0.0757	0.4187	0.0539	0.025
H(B3)	0.5548	0.6427	0.1437	0.023
H(B4)	0.7258	0.5845	0.2249	0.024
H(B5)	0.7630	0.1769	0.3710	0.023
H(B6)	0.6157	-0.0330	0.3891	0.023
H(B7)	0.1462	-0.2668	0.2832	0.023
H(B8)	-0.0252	-0.2064	0.2040	0.023
H(12)	0.3919	0.5215	-0.0182	0.028
H(13)	0.3823	0.6967	-0.0903	0.030
H(14)	0.3036	0.8517	-0.0354	0.028
H(15)	0.2227	0.8244	0.0891	0.029
H(16)	0.2290	0.6479	0.1604	0.027
H(22)	0.7564	0.4875	0.4038	0.034
H(23)	0.9697	0.5769	0.4465	0.047
H(24)	1.1345	0.5499	0.3728	0.048
H(25)	1.0871	0.4371	0.2557	0.049
H(26)	0.8747	0.3413	0.2143	0.035
H(32)	0.3478	-0.1308	0.4606	0.026
H(33)	0.3570	-0.3102	0.5276	0.030
H(34)	0.3979	-0.4780	0.4618	0.028
H(35)	0.4336	-0.4642	0.3281	0.032
H(36)	0.4252	-0.2840	0.2608	0.029
H(42)	-0.0722	-0.1132	0.0388	0.029
H(43)	-0.2886	-0.2010	0.0024	0.033
H(44)	-0.4462	-0.1572	0.0757	0.030
H(45)	-0.3884	-0.0321	0.1886	0.032
H(46)	-0.1726	0.0572	0.2246	0.027
H(1)	0.4283	0.2580	0.4000	0.028
H(2)	0.3384	0.2364	0.5195	0.033
H(4)	-0.0081	0.1807	0.4025	0.033
H(5)	0.0945	0.2033	0.2880	0.030
H(6A)	-0.0801	0.2125	0.5247	0.059
H(6B)	-0.0749	0.1232	0.5971	0.059

Table S6. Continued

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
H(6C)	-0.0816	0.0702	0.5095	0.059
H(7A)	0.1994	0.1106	0.6219	0.074
H(7B)	0.1083	0.1808	0.6623	0.074
H(7C)	0.2345	0.2597	0.6232	0.074

^a *U*(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor the estimated standard deviations of the least significant digits are given in parentheses.

Table S7. Complete Crystallographic Details for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.

formula	C49H35Cl ₃ FeN ₇ O
FW, amu	900.04
<i>a</i> , Å	17.5274(8)
<i>b</i> , Å	25.2009(11)
<i>c</i> , Å	9.6227(4)
β , deg	90
<i>V</i> , Å ³	4250.4(3)
space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>Z</i>	4
D _c , g/cm ³	1.407
F(000)	1852
μ , mm ⁻¹	0.591
crystal dimensions, mm	0.32 × 0.21 × 0.19
radiation	MoK α , $\bar{\lambda} = 0.71073$ Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.99–28.27
index range	$-23 \leq h \leq 23$ $-33 \leq k \leq 33$ $-12 \leq l \leq 12$
total data collected	46920
absorption correction	Empirical
relative transmission coefficients (I)	1.000 and 0.870
unique data	10522 ($R_{\text{int}} = 0.072$)
unique observed data [$I > 2\sigma(I)$]	9046
refinement method	Full-matrix least-squares on F ²
data/restraints/parameters	10522/0/558
goodness-of-fit (based on F ²)	1.070
final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.0518$, $wR_2 = 0.1092$
final <i>R</i> indices (all data)	$R_1 = 0.0637$, $wR_2 = 0.1155$

Table S8. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.^a

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
Fe(1)	0.09637(2)	0.16653(2)	0.27822(4)	0.0127(1)
N(1)	0.09318(14)	0.24389(9)	0.2331(2)	0.0160(5)
N(2)	0.21130(13)	0.17010(9)	0.2908(2)	0.0150(5)
N(3)	0.10068(15)	0.08916(9)	0.3321(2)	0.0147(5)
N(4)	-0.01737(13)	0.16393(9)	0.2829(2)	0.0157(5)
C(a1)	0.02902(17)	0.27405(11)	0.2060(3)	0.0160(6)
C(a2)	0.15368(17)	0.27687(11)	0.2099(3)	0.0182(6)
C(a3)	0.25683(17)	0.21439(11)	0.2702(3)	0.0159(6)
C(a4)	0.26098(17)	0.12872(12)	0.3150(3)	0.0157(6)
C(a5)	0.16482(17)	0.05798(11)	0.3405(3)	0.0151(6)
C(a6)	0.03947(17)	0.05455(12)	0.3416(3)	0.0161(6)
C(a7)	-0.06314(17)	0.12070(12)	0.3131(3)	0.0161(6)
C(a8)	-0.06686(17)	0.20602(12)	0.2655(3)	0.0167(6)
C(b1)	0.05059(18)	0.32632(12)	0.1628(3)	0.0201(6)
C(b2)	0.12761(17)	0.32835(12)	0.1649(3)	0.0191(6)
C(b3)	0.33577(17)	0.20046(11)	0.2907(3)	0.0170(6)
C(b4)	0.33866(18)	0.14789(12)	0.3166(3)	0.0181(6)
C(b5)	0.14370(17)	0.00265(12)	0.3532(3)	0.0171(6)
C(b6)	0.06740(18)	0.00072(12)	0.3550(3)	0.0178(6)
C(b7)	-0.14195(18)	0.13694(12)	0.3188(3)	0.0187(6)
C(b8)	-0.14421(17)	0.18917(12)	0.2898(3)	0.0191(6)
C(m1)	0.23071(16)	0.26460(11)	0.2317(3)	0.0156(6)
C(m2)	0.24031(17)	0.07590(12)	0.3349(3)	0.0148(6)
C(m3)	-0.03753(17)	0.06879(12)	0.3380(3)	0.0161(6)
C(m4)	-0.04637(17)	0.25749(11)	0.2263(3)	0.0168(6)
C(11)	0.28797(16)	0.30804(11)	0.2130(3)	0.0166(6)
C(12)	0.32665(18)	0.31563(13)	0.0878(3)	0.0218(7)
C(13)	0.37761(18)	0.35689(13)	0.0712(4)	0.0253(7)
C(14)	0.39092(17)	0.39150(13)	0.1818(4)	0.0262(7)
C(15)	0.35347(18)	0.38446(13)	0.3063(3)	0.0244(7)
C(16)	0.30199(18)	0.34282(12)	0.3223(3)	0.0218(7)
C(21)	0.30184(17)	0.03467(11)	0.3442(3)	0.0158(6)
C(22)	0.33902(17)	0.01745(12)	0.2248(3)	0.0194(6)
C(23)	0.39070(17)	-0.02428(13)	0.2303(3)	0.0232(6)

Table S8. Continued

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
C(24)	0.40702(19)	-0.04893(12)	0.3562(3)	0.0221(6)
C(25)	0.37223(17)	-0.03088(12)	0.4773(3)	0.0195(6)
C(26)	0.31939(17)	0.01050(12)	0.4715(3)	0.0192(6)
C(31)	-0.09599(19)	0.02683(11)	0.3616(3)	0.0176(6)
C(32)	-0.09871(19)	-0.00053(11)	0.4881(3)	0.0188(6)
C(33)	-0.15648(19)	-0.03732(12)	0.5140(4)	0.0240(7)
C(34)	-0.21105(18)	-0.04748(12)	0.4151(4)	0.0237(7)
C(35)	-0.20857(17)	-0.02148(13)	0.2874(4)	0.0244(7)
C(36)	-0.15100(18)	0.01521(12)	0.2610(3)	0.0218(7)
C(41)	-0.10914(16)	0.29746(11)	0.2074(3)	0.0165(6)
C(42)	-0.13325(18)	0.31343(12)	0.0757(3)	0.0192(6)
C(43)	-0.19257(18)	0.34921(12)	0.0601(3)	0.0221(7)
C(44)	-0.22893(18)	0.37008(12)	0.1770(3)	0.0215(7)
C(45)	-0.20391(19)	0.35568(13)	0.3080(3)	0.0232(7)
C(46)	-0.14498(18)	0.31945(12)	0.3234(3)	0.0215(7)
N(5)	0.09553(16)	0.15338(9)	0.0996(2)	0.0168(5)
O(1a)	0.06136(17)	0.16753(12)	0.0005(3)	0.0306(6)
O(1b)	0.1266(9)	0.1703(6)	-0.0022(16)	0.026(3)
N(6)	0.08949(14)	0.18908(9)	0.4958(2)	0.0169(5)
N(7)	0.11430(14)	0.22666(10)	0.6990(2)	0.0191(5)
C(1)	0.02654(19)	0.18560(15)	0.5803(3)	0.0281(8)
C(2)	0.04136(18)	0.20831(14)	0.7048(3)	0.0256(7)
C(3)	0.14091(18)	0.21438(12)	0.5705(3)	0.0206(6)
C(4)	0.1552(2)	0.25480(14)	0.8085(3)	0.0289(8)
Cl(1)	0.66180(6)	0.06624(5)	0.42591(11)	0.0521(3)
Cl(2)	0.57111(9)	0.16173(4)	0.45765(13)	0.0657(4)
Cl(3)	0.50669(6)	0.05996(5)	0.52423(13)	0.0523(3)
C(5)	0.5884(2)	0.09856(14)	0.5222(4)	0.0348(8)

^a *U*(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S9. Bond Lengths for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.^a

bond	length (Å)	bond	length (Å)
Fe(1)–N(5)	1.750(2)	C(m4)–C(41)	1.503(4)
Fe(1)–N(4)	1.995(2)	C(11)–C(16)	1.391(4)
Fe(1)–N(1)	1.998(2)	C(11)–C(12)	1.396(4)
Fe(1)–N(3)	2.019(2)	C(12)–C(13)	1.380(4)
Fe(1)–N(2)	2.020(2)	C(13)–C(14)	1.396(5)
Fe(1)–N(6)	2.173(2)	C(14)–C(15)	1.377(5)
N(1)–C(a2)	1.366(4)	C(15)–C(16)	1.393(4)
N(1)–C(a1)	1.382(4)	C(21)–C(22)	1.390(4)
N(2)–C(a4)	1.378(4)	C(21)–C(26)	1.402(4)
N(2)–C(a3)	1.386(4)	C(22)–C(23)	1.389(4)
N(3)–C(a5)	1.374(4)	C(23)–C(24)	1.391(4)
N(3)–C(a6)	1.386(4)	C(24)–C(25)	1.392(4)
N(4)–C(a8)	1.380(4)	C(25)–C(26)	1.396(4)
N(4)–C(a7)	1.384(4)	C(31)–C(36)	1.397(4)
C(a1)–C(m4)	1.400(4)	C(31)–C(32)	1.400(4)
C(a1)–C(b1)	1.432(4)	C(32)–C(33)	1.395(4)
C(a2)–C(m1)	1.401(4)	C(33)–C(34)	1.373(5)
C(a2)–C(b2)	1.442(4)	C(34)–C(35)	1.394(5)
C(a3)–C(m1)	1.396(4)	C(35)–C(36)	1.392(4)
C(a3)–C(b3)	1.441(4)	C(41)–C(42)	1.395(4)
C(a4)–C(m2)	1.393(4)	C(41)–C(46)	1.396(4)
C(a4)–C(b4)	1.445(4)	C(42)–C(43)	1.384(4)
C(a5)–C(m2)	1.399(4)	C(43)–C(44)	1.396(4)
C(a5)–C(b5)	1.448(4)	C(44)–C(45)	1.383(5)
C(a6)–C(m3)	1.397(4)	C(45)–C(46)	1.386(4)
C(a6)–C(b6)	1.448(4)	N(5)–O(1a)	1.182(3)
C(a7)–C(m3)	1.404(4)	N(5)–O(1b)	1.199(15)
C(a7)–C(b7)	1.442(4)	N(6)–C(3)	1.318(4)
C(a8)–C(m4)	1.398(4)	N(6)–C(1)	1.374(4)
C(a8)–C(b8)	1.440(4)	N(7)–C(3)	1.357(4)
C(b1)–C(b2)	1.351(4)	N(7)–C(2)	1.361(4)
C(b3)–C(b4)	1.349(4)	N(7)–C(4)	1.458(4)
C(b5)–C(b6)	1.338(4)	C(1)–C(2)	1.353(4)
C(b7)–C(b8)	1.346(4)	Cl(1)–C(5)	1.782(4)

Table S9. Continued

bond	length (Å)	bond	length (Å)
C(m1)–C(11)	1.496(4)	Cl(2)–C(5)	1.736(4)
C(m2)–C(21)	1.500(4)	Cl(3)–C(5)	1.732(4)
C(m3)–C(31)	1.490(4)		

^aThe estimated standard deviations of the least significant digits are given in parentheses.

Table S10. Bond Angles for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.^a

angle	degree	angle	degree
N(5)–Fe(1)–N(4)	90.43(11)	C(a3)–C(m1)–C(11)	118.4(3)
N(5)–Fe(1)–N(1)	88.34(10)	C(a2)–C(m1)–C(11)	117.9(3)
N(4)–Fe(1)–N(1)	90.52(10)	C(a4)–C(m2)–C(a5)	124.0(3)
N(5)–Fe(1)–N(3)	93.99(10)	C(a4)–C(m2)–C(21)	118.9(3)
N(4)–Fe(1)–N(3)	89.99(10)	C(a5)–C(m2)–C(21)	117.0(3)
N(1)–Fe(1)–N(3)	177.61(10)	C(a6)–C(m3)–C(a7)	123.5(3)
N(5)–Fe(1)–N(2)	94.34(11)	C(a6)–C(m3)–C(31)	118.6(3)
N(4)–Fe(1)–N(2)	175.22(9)	C(a7)–C(m3)–C(31)	117.9(3)
N(1)–Fe(1)–N(2)	89.85(10)	C(a8)–C(m4)–C(a1)	123.9(3)
N(3)–Fe(1)–N(2)	89.45(10)	C(a8)–C(m4)–C(41)	117.8(3)
N(5)–Fe(1)–N(6)	174.37(11)	C(a1)–C(m4)–C(41)	118.3(3)
N(4)–Fe(1)–N(6)	86.07(10)	C(16)–C(11)–C(12)	118.7(3)
N(1)–Fe(1)–N(6)	87.28(9)	C(16)–C(11)–C(m1)	119.3(3)
N(3)–Fe(1)–N(6)	90.42(9)	C(12)–C(11)–C(m1)	122.0(3)
N(2)–Fe(1)–N(6)	89.19(10)	C(13)–C(12)–C(11)	121.2(3)
C(a2)–N(1)–C(a1)	105.4(2)	C(12)–C(13)–C(14)	119.4(3)
C(a2)–N(1)–Fe(1)	127.4(2)	C(15)–C(14)–C(13)	120.2(3)
C(a1)–N(1)–Fe(1)	126.9(2)	C(14)–C(15)–C(16)	120.1(3)
C(a4)–N(2)–C(a3)	105.6(2)	C(11)–C(16)–C(15)	120.4(3)
C(a4)–N(2)–Fe(1)	127.3(2)	C(22)–C(21)–C(26)	118.9(3)
C(a3)–N(2)–Fe(1)	126.97(19)	C(22)–C(21)–C(m2)	120.3(3)
C(a5)–N(3)–C(a6)	105.6(2)	C(26)–C(21)–C(m2)	120.7(3)
C(a5)–N(3)–Fe(1)	126.7(2)	C(23)–C(22)–C(21)	120.7(3)
C(a6)–N(3)–Fe(1)	126.6(2)	C(22)–C(23)–C(24)	120.4(3)
C(a8)–N(4)–C(a7)	105.4(2)	C(23)–C(24)–C(25)	119.5(3)
C(a8)–N(4)–Fe(1)	126.9(2)	C(24)–C(25)–C(26)	120.1(3)
C(a7)–N(4)–Fe(1)	127.58(19)	C(25)–C(26)–C(21)	120.3(3)
N(1)–C(a1)–C(m4)	125.3(3)	C(36)–C(31)–C(32)	118.4(3)
N(1)–C(a1)–C(b1)	110.2(3)	C(36)–C(31)–C(m3)	121.2(3)
C(m4)–C(a1)–C(b1)	124.3(3)	C(32)–C(31)–C(m3)	120.4(3)
N(1)–C(a2)–C(m1)	126.1(3)	C(33)–C(32)–C(31)	120.5(3)
N(1)–C(a2)–C(b2)	110.5(3)	C(34)–C(33)–C(32)	120.4(3)
C(m1)–C(a2)–C(b2)	123.3(3)	C(33)–C(34)–C(35)	120.1(3)
N(2)–C(a3)–C(m1)	125.4(3)	C(36)–C(35)–C(34)	119.7(3)

Table S10. Continued

angle	degree	angle	degree
N(2)–C(a3)–C(b3)	109.7(2)	C(35)–C(36)–C(31)	120.8(3)
C(m1)–C(a3)–C(b3)	124.9(3)	C(42)–C(41)–C(46)	118.4(3)
N(2)–C(a4)–C(m2)	125.6(3)	C(42)–C(41)–C(m4)	121.7(3)
N(2)–C(a4)–C(b4)	110.1(3)	C(46)–C(41)–C(m4)	119.9(3)
C(m2)–C(a4)–C(b4)	124.3(3)	C(43)–C(42)–C(41)	120.9(3)
N(3)–C(a5)–C(m2)	125.9(3)	C(42)–C(43)–C(44)	120.1(3)
N(3)–C(a5)–C(b5)	110.3(3)	C(45)–C(44)–C(43)	119.4(3)
C(m2)–C(a5)–C(b5)	123.8(3)	C(44)–C(45)–C(46)	120.4(3)
N(3)–C(a6)–C(m3)	125.8(3)	C(45)–C(46)–C(41)	120.8(3)
N(3)–C(a6)–C(b6)	109.5(3)	O(1a)–N(5)–O(1b)	57.5(7)
C(m3)–C(a6)–C(b6)	124.7(3)	O(1a)–N(5)–Fe(1)	137.7(2)
N(4)–C(a7)–C(m3)	125.7(3)	O(1b)–N(5)–Fe(1)	137.0(8)
N(4)–C(a7)–C(b7)	109.9(3)	C(3)–N(6)–C(1)	104.9(3)
C(m3)–C(a7)–C(b7)	124.4(3)	C(3)–N(6)–Fe(1)	127.9(2)
N(4)–C(a8)–C(m4)	125.8(3)	C(1)–N(6)–Fe(1)	126.8(2)
N(4)–C(a8)–C(b8)	110.2(3)	C(3)–N(7)–C(2)	106.4(3)
C(m4)–C(a8)–C(b8)	124.0(3)	C(3)–N(7)–C(4)	126.9(3)
C(b2)–C(b1)–C(a1)	107.1(3)	C(2)–N(7)–C(4)	126.7(3)
C(b1)–C(b2)–C(a2)	106.7(3)	C(2)–C(1)–N(6)	110.1(3)
C(b4)–C(b3)–C(a3)	107.5(3)	C(1)–C(2)–N(7)	106.8(3)
C(b3)–C(b4)–C(a4)	106.9(3)	N(6)–C(3)–N(7)	111.9(3)
C(b6)–C(b5)–C(a5)	106.9(3)	Cl(3)–C(5)–Cl(2)	112.0(2)
C(b5)–C(b6)–C(a6)	107.6(3)	Cl(3)–C(5)–Cl(1)	110.25(19)
C(b8)–C(b7)–C(a7)	107.3(3)	Cl(2)–C(5)–Cl(1)	111.1(2)
C(b7)–C(b8)–C(a8)	107.1(3)		
C(a3)–C(m1)–C(a2)	123.8(3)		

^aThe estimated standard deviations of the least significant digits are given in parentheses.

Table S11. Anisotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.^a

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0146(2)	0.0118(2)	0.0119(2)	0.0005(2)	-0.0007(2)	0.0001(2)
N(1)	0.0176(11)	0.0151(11)	0.0153(11)	-0.0010(9)	0.0001(11)	-0.0003(10)
N(2)	0.0175(11)	0.0142(12)	0.0132(11)	0.0005(11)	0.0001(10)	0.0003(9)
N(3)	0.0174(12)	0.0149(11)	0.0117(10)	0.0008(9)	0.0019(10)	-0.0007(10)
N(4)	0.0189(12)	0.0127(11)	0.0155(11)	0.0002(11)	-0.0014(10)	0.0003(10)
C(A1)	0.0225(15)	0.0130(13)	0.0126(14)	-0.0002(11)	-0.0018(12)	0.0004(11)
C(A2)	0.0242(15)	0.0168(14)	0.0134(14)	-0.0011(12)	-0.0009(13)	-0.0023(12)
C(A3)	0.0210(14)	0.0187(14)	0.0081(12)	-0.0022(11)	0.0003(12)	-0.0020(11)
C(A4)	0.0188(14)	0.0194(15)	0.0089(13)	-0.0020(11)	0.0006(11)	0.0022(12)
C(A5)	0.0210(15)	0.0141(14)	0.0101(13)	0.0005(11)	0.0013(11)	0.0032(12)
C(A6)	0.0212(15)	0.0159(14)	0.0113(13)	-0.0005(11)	0.0004(11)	0.0006(12)
C(A7)	0.0194(14)	0.0151(14)	0.0138(14)	0.0001(11)	-0.0015(11)	0.0002(11)
C(A8)	0.0207(14)	0.0150(13)	0.0145(14)	-0.0013(12)	-0.0030(12)	0.0019(11)
C(B1)	0.0228(16)	0.0170(15)	0.0204(15)	0.0012(12)	-0.0009(12)	0.0006(12)
C(B2)	0.0236(15)	0.0152(15)	0.0186(14)	-0.0014(12)	0.0011(12)	-0.0006(12)
C(B3)	0.0200(14)	0.0175(14)	0.0134(14)	-0.0029(12)	0.0001(12)	-0.0042(11)
C(B4)	0.0165(14)	0.0234(15)	0.0144(13)	-0.0017(11)	-0.0005(11)	-0.0007(12)
C(B5)	0.0199(15)	0.0153(14)	0.0162(14)	0.0001(12)	-0.0022(11)	0.0021(12)
C(B6)	0.0220(15)	0.0136(14)	0.0180(14)	0.0013(12)	0.0005(12)	0.0002(12)
C(B7)	0.0180(15)	0.0183(15)	0.0199(15)	0.0009(12)	-0.0001(12)	-0.0018(12)
C(B8)	0.0181(15)	0.0205(15)	0.0186(15)	0.0013(13)	0.0022(13)	0.0037(11)
C(M1)	0.0190(14)	0.0155(13)	0.0123(13)	-0.0016(11)	0.0045(12)	-0.0013(11)
C(M2)	0.0181(14)	0.0174(14)	0.0089(13)	-0.0006(11)	-0.0008(11)	0.0027(11)
C(M3)	0.0189(15)	0.0156(14)	0.0137(13)	0.0010(11)	-0.0023(11)	-0.0030(11)
C(M4)	0.0214(14)	0.0151(14)	0.0139(13)	-0.0005(12)	-0.0023(12)	0.0026(11)
C(11)	0.0157(13)	0.0127(13)	0.0213(15)	0.0022(12)	-0.0005(12)	0.0012(10)
C(12)	0.0236(16)	0.0197(15)	0.0220(16)	-0.0022(13)	0.0026(13)	0.0011(12)
C(13)	0.0208(16)	0.0282(18)	0.0268(17)	0.0054(14)	0.0081(13)	0.0021(13)
C(14)	0.0149(16)	0.0221(16)	0.0415(19)	0.0044(14)	-0.0038(14)	-0.0035(12)
C(15)	0.0232(16)	0.0230(16)	0.0270(17)	-0.0007(13)	-0.0081(13)	-0.0034(13)
C(16)	0.0223(16)	0.0229(17)	0.0203(14)	-0.0003(12)	-0.0022(12)	-0.0015(12)
C(21)	0.0157(14)	0.0131(14)	0.0186(14)	0.0020(11)	-0.0029(12)	-0.0010(11)
C(22)	0.0210(15)	0.0219(15)	0.0154(13)	0.0023(13)	0.0019(13)	0.0030(12)
C(23)	0.0205(16)	0.0264(16)	0.0227(14)	0.0026(13)	0.0065(13)	0.0044(12)

Table S11. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	0.0168(14)	0.0202(15)	0.0292(16)	0.0047(12)	0.0021(14)	0.0023(13)
C(25)	0.0217(15)	0.0198(16)	0.0169(14)	0.0026(12)	-0.0041(12)	-0.0023(12)
C(26)	0.0223(16)	0.0182(16)	0.0172(14)	0.0003(12)	0.0017(12)	-0.0014(12)
C(31)	0.0192(14)	0.0116(13)	0.0220(14)	-0.0003(11)	-0.0004(13)	0.0035(13)
C(32)	0.0214(14)	0.0154(13)	0.0197(14)	-0.0021(11)	0.0026(14)	0.0015(13)
C(33)	0.0284(17)	0.0159(15)	0.0277(17)	0.0022(13)	0.0081(14)	0.0041(13)
C(34)	0.0198(16)	0.0121(15)	0.0393(19)	0.0001(14)	0.0060(14)	-0.0003(12)
C(35)	0.0170(15)	0.0219(15)	0.0344(18)	-0.0062(15)	-0.0035(15)	0.0004(12)
C(36)	0.0245(16)	0.0171(14)	0.0240(16)	-0.0011(12)	-0.0007(13)	0.0024(12)
C(41)	0.0165(14)	0.0121(12)	0.0209(15)	0.0008(11)	-0.0030(12)	-0.0018(11)
C(42)	0.0212(16)	0.0203(15)	0.0160(14)	0.0002(12)	-0.0008(12)	0.0027(12)
C(43)	0.0245(16)	0.0224(16)	0.0193(15)	0.0055(13)	-0.0026(13)	0.0033(13)
C(44)	0.0220(16)	0.0134(14)	0.0290(17)	0.0024(12)	0.0004(13)	0.0019(12)
C(45)	0.0278(17)	0.0206(16)	0.0210(16)	-0.0016(12)	0.0032(13)	-0.0001(13)
C(46)	0.0278(17)	0.0228(16)	0.0140(13)	0.0022(12)	-0.0047(12)	0.0011(13)
N(5)	0.0220(12)	0.0148(12)	0.0135(11)	-0.0015(9)	-0.0007(11)	0.0012(11)
O(1A)	0.0442(17)	0.0301(15)	0.0176(13)	0.0010(12)	-0.0080(12)	0.0093(14)
N(6)	0.0200(13)	0.0150(11)	0.0158(11)	0.0020(9)	-0.0011(11)	0.0007(10)
N(7)	0.0230(14)	0.0212(13)	0.0132(12)	-0.0029(10)	-0.0026(10)	0.0003(10)
C(1)	0.0200(16)	0.045(2)	0.0188(15)	-0.0023(15)	0.0012(13)	-0.0124(15)
C(2)	0.0225(16)	0.0394(19)	0.0149(15)	0.0014(14)	0.0027(13)	-0.0041(14)
C(3)	0.0193(15)	0.0247(17)	0.0179(15)	-0.0007(13)	0.0011(12)	0.0001(12)
C(4)	0.0339(19)	0.036(2)	0.0168(15)	-0.0065(14)	-0.0038(14)	-0.0048(16)
Cl(1)	0.0451(6)	0.0738(8)	0.0373(5)	-0.0116(5)	0.0101(5)	0.0035(6)
Cl(2)	0.1125(11)	0.0311(5)	0.0534(7)	0.0050(5)	0.0188(7)	-0.0090(6)
Cl(3)	0.0366(5)	0.0504(6)	0.0698(8)	0.0175(6)	-0.0008(5)	-0.0131(5)
C(5)	0.043(2)	0.0315(18)	0.0300(18)	-0.0033(15)	0.0105(17)	-0.0085(17)

^aThe estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2 \pi [h^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Table S12. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.^a

atom	x	y	z	U(eq)
H(B1)	0.0170	0.3543	0.1374	0.024
H(B2)	0.1586	0.3579	0.1413	0.023
H(B3)	0.3780	0.2240	0.2867	0.020
H(B4)	0.3833	0.1274	0.3327	0.022
H(B5)	0.1776	-0.0267	0.3591	0.021
H(B6)	0.0371	-0.0303	0.3635	0.021
H(B7)	-0.1844	0.1149	0.3391	0.022
H(B8)	-0.1885	0.2108	0.2861	0.023
H(12)	0.3177	0.2920	0.0126	0.026
H(13)	0.4034	0.3617	-0.0147	0.030
H(14)	0.4259	0.4200	0.1712	0.031
H(15)	0.3628	0.4081	0.3814	0.029
H(16)	0.2763	0.3381	0.4083	0.026
H(22)	0.3290	0.0344	0.1386	0.023
H(23)	0.4150	-0.0360	0.1477	0.028
H(24)	0.4417	-0.0779	0.3594	0.026
H(25)	0.3845	-0.0468	0.5640	0.023
H(26)	0.2952	0.0223	0.5542	0.023
H(32)	-0.0609	0.0060	0.5568	0.023
H(33)	-0.1581	-0.0554	0.6005	0.029
H(34)	-0.2506	-0.0723	0.4339	0.028
H(35)	-0.2460	-0.0288	0.2186	0.029
H(36)	-0.1491	0.0326	0.1734	0.026
H(42)	-0.1086	0.2996	-0.0044	0.023
H(43)	-0.2085	0.3596	-0.0303	0.026
H(44)	-0.2705	0.3940	0.1667	0.026
H(45)	-0.2273	0.3707	0.3879	0.028
H(46)	-0.1288	0.3095	0.4139	0.026
H(1)	-0.0205	0.1696	0.5551	0.034
H(2)	0.0074	0.2109	0.7814	0.031
H(3)	0.1906	0.2230	0.5384	0.025
H(4A)	0.2019	0.2354	0.8317	0.043
H(4B)	0.1227	0.2574	0.8911	0.043
H(4C)	0.1684	0.2905	0.7761	0.043

Table S12. Continued

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
H(5)	0.6065	0.1024	0.6203	0.042

^a U (eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor the estimated standard deviations of the least significant digits are given in parentheses.

Table S13. Complete Crystallographic Details for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.

formula	C ₅₀ H ₄₀ Cl ₃ FeN ₇ O
FW, amu	917.09
<i>a</i> , Å	17.6359(7)
<i>b</i> , Å	25.2877(10)
<i>c</i> , Å	9.9670(4)
β , deg	90
<i>V</i> , Å ³	4445.0(3)
space group	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>Z</i>	4
D _c , g/cm ³	1.370
F(000)	1896
μ , mm ⁻¹	0.566
crystal dimensions, mm	0.28 × 0.20 × 0.19
radiation	MoK α , $\bar{\lambda} = 0.71073$ Å
temperature, K	100(2)
diffractometer	Bruker Apex CCD
θ range for collected data, deg	1.98–28.29
index range	$-23 \leq h \leq 23$ $-33 \leq k \leq 33$ $-13 \leq l \leq 13$
total data collected	49041
absorption correction	Empirical
relative transmission coefficients (I)	1.0000 and 0.8955
unique data	11029 ($R_{\text{int}} = 0.030$)
unique observed data [$I > 2\sigma(I)$]	10485
refinement method	Full-matrix least-squares on F ²
data/restraints/parameters	11029/0/596
goodness-of-fit (based on F ²)	1.046
final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.0411$, $wR_2 = 0.1085$
final <i>R</i> indices (all data)	$R_1 = 0.0433$, $wR_2 = 0.1105$

Table S14. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.^a

atom	x	y	z	U(eq)
Fe(1)	0.91228(2)	0.16976(1)	0.72058(3)	0.0173(1)
N(1)	0.79828(9)	0.17226(6)	0.73525(17)	0.0188(3)
N(2)	0.91672(10)	0.24793(6)	0.75637(17)	0.0211(3)
N(3)	1.02421(9)	0.16895(7)	0.69086(17)	0.0194(3)
N(4)	0.90610(10)	0.09283(6)	0.67070(17)	0.0190(3)
C(a1)	0.74829(11)	0.13088(8)	0.7210(2)	0.0197(4)
C(a2)	0.75401(11)	0.21568(8)	0.7639(2)	0.0193(4)
C(a3)	0.85709(11)	0.28134(8)	0.7842(2)	0.0222(4)
C(a4)	0.98071(11)	0.27932(8)	0.7613(2)	0.0225(4)
C(a5)	1.07369(11)	0.21085(8)	0.7000(2)	0.0198(4)
C(a6)	1.06854(11)	0.12557(8)	0.6614(2)	0.0204(4)
C(a7)	0.96660(12)	0.05897(8)	0.6546(2)	0.0202(4)
C(a8)	0.84266(11)	0.06119(8)	0.6760(2)	0.0191(4)
C(b1)	0.67115(11)	0.14910(8)	0.7369(2)	0.0226(4)
C(b2)	0.67479(11)	0.20158(8)	0.7635(2)	0.0222(4)
C(b3)	0.88391(13)	0.33447(9)	0.8062(2)	0.0273(5)
C(b4)	0.95999(12)	0.33310(8)	0.7919(2)	0.0264(4)
C(b5)	1.14969(12)	0.19402(8)	0.6706(2)	0.0229(4)
C(b6)	1.14700(12)	0.14120(8)	0.6459(2)	0.0229(4)
C(b7)	0.94032(12)	0.00469(8)	0.6503(2)	0.0225(4)
C(b8)	0.86391(12)	0.00616(8)	0.6626(2)	0.0217(4)
C(m1)	0.78073(11)	0.26703(8)	0.7889(2)	0.0216(4)
C(m2)	1.05451(11)	0.26261(8)	0.7343(2)	0.0213(4)
C(m3)	1.04244(12)	0.07356(8)	0.6457(2)	0.0215(4)
C(m4)	0.76805(11)	0.07836(8)	0.6948(2)	0.0193(4)
C(11)	0.72317(11)	0.30907(8)	0.8193(2)	0.0213(4)
C(12)	0.69357(12)	0.31455(9)	0.9476(2)	0.0243(4)
C(13)	0.63891(12)	0.35353(9)	0.9741(2)	0.0264(4)
C(14)	0.61496(12)	0.38670(9)	0.8723(3)	0.0270(5)
C(15)	0.64421(13)	0.38134(9)	0.7434(3)	0.0297(5)
C(16)	0.69819(12)	0.34249(9)	0.7176(3)	0.0271(4)
C(21)	1.11744(11)	0.30249(8)	0.7450(2)	0.0218(4)
C(22)	1.14746(13)	0.32606(9)	0.6312(2)	0.0268(4)
C(23)	1.20591(14)	0.36310(9)	0.6419(3)	0.0295(5)

Table S14. Continued

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
C(24)	1.23428(12)	0.37682(8)	0.7664(3)	0.0276(5)
C(25)	1.20517(14)	0.35295(10)	0.8816(3)	0.0297(5)
C(26)	1.14646(13)	0.31629(8)	0.8702(2)	0.0249(4)
C(31)	1.10026(12)	0.03134(8)	0.6190(3)	0.0248(4)
C(32)	1.10082(13)	0.00473(9)	0.4962(3)	0.0296(5)
C(33)	1.15576(15)	-0.03410(10)	0.4699(3)	0.0383(6)
C(34)	1.20872(15)	-0.04599(10)	0.5651(4)	0.0416(7)
C(35)	1.20870(14)	-0.02061(10)	0.6881(4)	0.0410(7)
C(36)	1.15431(13)	0.01835(9)	0.7154(3)	0.0335(5)
C(41)	0.70626(11)	0.03760(8)	0.6876(2)	0.0198(4)
C(42)	0.68977(12)	0.01274(8)	0.5655(2)	0.0242(4)
C(43)	0.63313(12)	-0.02548(9)	0.5578(2)	0.0255(4)
C(44)	0.59271(12)	-0.03961(8)	0.6717(2)	0.0247(4)
C(45)	0.60869(11)	-0.01533(8)	0.7942(2)	0.0241(4)
C(46)	0.66484(12)	0.02368(8)	0.8015(2)	0.0222(4)
N(5)	0.92770(10)	0.15043(7)	0.88713(19)	0.0222(4)
O(1)	0.96777(9)	0.12179(7)	0.94635(18)	0.0313(4)
N(6)	0.89556(10)	0.18775(7)	0.49786(18)	0.0216(3)
C(1)	0.86788(14)	0.24260(9)	0.4710(2)	0.0272(5)
C(2)	0.85350(13)	0.25397(9)	0.3237(2)	0.0286(5)
C(3)	0.94675(15)	0.18569(10)	0.2629(2)	0.0327(5)
C(4)	0.96143(13)	0.17483(9)	0.4105(2)	0.0278(4)
N(7)	0.92380(14)	0.24368(9)	0.2402(2)	0.0429(5)
C(5)	0.9097(2)	0.25529(12)	0.0926(3)	0.0453(7)
Cl(1)	0.48613(6)	0.04947(4)	0.43373(12)	0.0443(2)
Cl(2)	0.33656(6)	0.06106(6)	0.54590(13)	0.0529(3)
Cl(3)	0.46180(9)	0.11438(8)	0.66808(19)	0.0650(4)
C(6)	0.4235(2)	0.09128(15)	0.5177(4)	0.0302(7)
Cl(1a)	0.46488(17)	0.11098(13)	0.7712(6)	0.0958(14)
Cl(2a)	0.3885(3)	0.03214(16)	0.6177(5)	0.1104(16)
Cl(3a)	0.4670(3)	0.11531(19)	0.4911(5)	0.1207(17)
C(6a)	0.4689(6)	0.0763(4)	0.6473(17)	0.079(4)

^a *U*(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S15. Bond Lengths for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.^a

bond	length (Å)	bond	length (Å)
Fe(1)–N(5)	1.7517(19)	C(11)–C(16)	1.391(3)
Fe(1)–N(3)	1.9962(16)	C(12)–C(13)	1.404(3)
Fe(1)–N(2)	2.0101(16)	C(13)–C(14)	1.382(3)
Fe(1)–N(4)	2.0109(16)	C(14)–C(15)	1.391(4)
Fe(1)–N(1)	2.0168(16)	C(15)–C(16)	1.392(3)
Fe(1)–N(6)	2.2851(19)	C(21)–C(22)	1.387(3)
N(1)–C(a1)	1.376(2)	C(21)–C(26)	1.393(3)
N(1)–C(a2)	1.377(2)	C(22)–C(23)	1.397(3)
N(2)–C(a3)	1.377(3)	C(23)–C(24)	1.382(4)
N(2)–C(a4)	1.381(2)	C(24)–C(25)	1.395(4)
N(3)–C(a5)	1.376(2)	C(25)–C(26)	1.394(3)
N(3)–C(a6)	1.379(3)	C(31)–C(36)	1.393(3)
N(4)–C(a8)	1.376(2)	C(31)–C(32)	1.397(3)
N(4)–C(a7)	1.377(3)	C(32)–C(33)	1.404(3)
C(a1)–C(m4)	1.397(3)	C(33)–C(34)	1.366(5)
C(a1)–C(b1)	1.445(3)	C(34)–C(35)	1.383(5)
C(a2)–C(m1)	1.404(3)	C(35)–C(36)	1.402(3)
C(a2)–C(b2)	1.442(3)	C(41)–C(46)	1.395(3)
C(a3)–C(m1)	1.395(3)	C(41)–C(42)	1.400(3)
C(a3)–C(b3)	1.441(3)	C(42)–C(43)	1.392(3)
C(a4)–C(m2)	1.395(3)	C(43)–C(44)	1.387(3)
C(a4)–C(b4)	1.441(3)	C(44)–C(45)	1.395(3)
C(a5)–C(m2)	1.394(3)	C(45)–C(46)	1.400(3)
C(a5)–C(b5)	1.437(3)	N(5)–O(1)	1.171(2)
C(a6)–C(m3)	1.402(3)	N(6)–C(4)	1.488(3)
C(a6)–C(b6)	1.447(3)	N(6)–C(1)	1.495(3)
C(a7)–C(m3)	1.390(3)	C(1)–C(2)	1.517(3)
C(a7)–C(b7)	1.450(3)	C(2)–N(7)	1.516(3)
C(a8)–C(m4)	1.398(3)	C(3)–C(4)	1.519(3)
C(a8)–C(b8)	1.447(3)	C(3)–N(7)	1.538(3)
C(b1)–C(b2)	1.355(3)	N(7)–C(5)	1.521(4)
C(b3)–C(b4)	1.350(3)	Cl(1)–C(6)	1.743(4)
C(b5)–C(b6)	1.359(3)	Cl(2)–C(6)	1.736(4)
C(b7)–C(b8)	1.354(3)	Cl(3)–C(6)	1.745(4)

Table S15. Continued

bond	length (Å)	bond	length (Å)
C(m1)–C(11)	1.501(3)	Cl(1a)–C(6a)	1.516(17)
C(m2)–C(21)	1.503(3)	Cl(2a)–C(6a)	1.830(13)
C(m3)–C(31)	1.500(3)	Cl(3a)–C(6a)	1.843(14)
C(m4)–C(41)	1.502(3)		
C(11)–C(12)	1.388(3)		

^aThe estimated standard deviations of the least significant digits are given in parentheses.

Table S16. Bond Angles for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.^a

angle	degree	angle	degree
N(5)–Fe(1)–N(3)	89.10(8)	C(a2)–C(m1)–C(11)	117.65(17)
N(5)–Fe(1)–N(2)	95.75(8)	C(a5)–C(m2)–C(a4)	123.92(18)
N(3)–Fe(1)–N(2)	89.88(7)	C(a5)–C(m2)–C(21)	117.91(17)
N(5)–Fe(1)–N(4)	88.44(8)	C(a4)–C(m2)–C(21)	118.16(18)
N(3)–Fe(1)–N(4)	90.39(7)	C(a7)–C(m3)–C(a6)	123.89(19)
N(2)–Fe(1)–N(4)	175.81(7)	C(a7)–C(m3)–C(31)	118.46(17)
N(5)–Fe(1)–N(1)	95.44(8)	C(a6)–C(m3)–C(31)	117.65(18)
N(3)–Fe(1)–N(1)	175.46(7)	C(a1)–C(m4)–C(a8)	123.70(18)
N(2)–Fe(1)–N(1)	89.73(7)	C(a1)–C(m4)–C(41)	118.71(17)
N(4)–Fe(1)–N(1)	89.67(7)	C(a8)–C(m4)–C(41)	117.59(18)
N(5)–Fe(1)–N(6)	174.98(7)	C(12)–C(11)–C(16)	119.4(2)
N(3)–Fe(1)–N(6)	89.17(7)	C(12)–C(11)–C(m1)	120.72(19)
N(2)–Fe(1)–N(6)	88.95(7)	C(16)–C(11)–C(m1)	119.8(2)
N(4)–Fe(1)–N(6)	86.87(7)	C(11)–C(12)–C(13)	120.1(2)
N(1)–Fe(1)–N(6)	86.30(7)	C(14)–C(13)–C(12)	119.8(2)
C(a1)–N(1)–C(a2)	105.35(15)	C(13)–C(14)–C(15)	120.4(2)
C(a1)–N(1)–Fe(1)	127.41(13)	C(14)–C(15)–C(16)	119.5(2)
C(a2)–N(1)–Fe(1)	127.24(13)	C(11)–C(16)–C(15)	120.7(2)
C(a3)–N(2)–C(a4)	105.32(16)	C(22)–C(21)–C(26)	119.02(18)
C(a3)–N(2)–Fe(1)	127.54(13)	C(22)–C(21)–C(m2)	120.78(19)
C(a4)–N(2)–Fe(1)	127.12(13)	C(26)–C(21)–C(m2)	120.21(19)
C(a5)–N(3)–C(a6)	105.50(15)	C(21)–C(22)–C(23)	120.5(2)
C(a5)–N(3)–Fe(1)	127.55(13)	C(24)–C(23)–C(22)	120.3(2)
C(a6)–N(3)–Fe(1)	126.92(13)	C(23)–C(24)–C(25)	119.80(19)
C(a8)–N(4)–C(a7)	105.83(15)	C(26)–C(25)–C(24)	119.6(2)
C(a8)–N(4)–Fe(1)	126.64(13)	C(21)–C(26)–C(25)	120.8(2)
C(a7)–N(4)–Fe(1)	126.02(13)	C(36)–C(31)–C(32)	119.1(2)
N(1)–C(a1)–C(m4)	125.62(17)	C(36)–C(31)–C(m3)	120.7(2)
N(1)–C(a1)–C(b1)	110.45(17)	C(32)–C(31)–C(m3)	120.2(2)
C(m4)–C(a1)–C(b1)	123.93(18)	C(31)–C(32)–C(33)	120.4(2)
N(1)–C(a2)–C(m1)	125.74(18)	C(34)–C(33)–C(32)	119.7(3)
N(1)–C(a2)–C(b2)	110.59(17)	C(33)–C(34)–C(35)	120.9(2)
C(m1)–C(a2)–C(b2)	123.67(18)	C(34)–C(35)–C(36)	119.9(3)
N(2)–C(a3)–C(m1)	125.78(18)	C(31)–C(36)–C(35)	120.0(3)

Table S16. Continued

angle	degree	angle	degree
N(2)–C(a3)–C(b3)	110.61(17)	C(46)–C(41)–C(42)	119.01(18)
C(m1)–C(a3)–C(b3)	123.61(19)	C(46)–C(41)–C(m4)	120.92(18)
N(2)–C(a4)–C(m2)	125.58(18)	C(42)–C(41)–C(m4)	120.08(18)
N(2)–C(a4)–C(b4)	110.05(17)	C(43)–C(42)–C(41)	120.6(2)
C(m2)–C(a4)–C(b4)	124.30(18)	C(44)–C(43)–C(42)	120.1(2)
N(3)–C(a5)–C(m2)	125.83(18)	C(43)–C(44)–C(45)	119.92(19)
N(3)–C(a5)–C(b5)	110.49(17)	C(44)–C(45)–C(46)	119.9(2)
C(m2)–C(a5)–C(b5)	123.67(18)	C(41)–C(46)–C(45)	120.4(2)
N(3)–C(a6)–C(m3)	125.72(18)	O(1)–N(5)–Fe(1)	138.04(17)
N(3)–C(a6)–C(b6)	110.34(17)	C(4)–N(6)–C(1)	110.71(17)
C(m3)–C(a6)–C(b6)	123.93(19)	C(4)–N(6)–Fe(1)	115.10(13)
N(4)–C(a7)–C(m3)	126.00(18)	C(1)–N(6)–Fe(1)	113.65(13)
N(4)–C(a7)–C(b7)	110.15(17)	N(6)–C(1)–C(2)	113.84(18)
C(m3)–C(a7)–C(b7)	123.84(18)	N(7)–C(2)–C(1)	111.21(19)
N(4)–C(a8)–C(m4)	126.13(18)	C(4)–C(3)–N(7)	111.1(2)
N(4)–C(a8)–C(b8)	110.17(17)	N(6)–C(4)–C(3)	113.21(18)
C(m4)–C(a8)–C(b8)	123.68(18)	C(2)–N(7)–C(5)	111.4(2)
C(b2)–C(b1)–C(a1)	106.81(18)	C(2)–N(7)–C(3)	107.4(2)
C(b1)–C(b2)–C(a2)	106.77(18)	C(5)–N(7)–C(3)	111.7(2)
C(b4)–C(b3)–C(a3)	106.64(19)	Cl(2)–C(6)–Cl(1)	111.7(2)
C(b3)–C(b4)–C(a4)	107.38(19)	Cl(2)–C(6)–Cl(3)	110.5(2)
C(b6)–C(b5)–C(a5)	107.19(19)	Cl(1)–C(6)–Cl(3)	111.7(2)
C(b5)–C(b6)–C(a6)	106.41(19)	Cl(1a)–C(6a)–Cl(2a)	116.6(7)
C(b8)–C(b7)–C(a7)	106.83(19)	Cl(1a)–C(6a)–Cl(3a)	112.2(6)
C(b7)–C(b8)–C(a8)	107.01(18)	Cl(2a)–C(6a)–Cl(3a)	100.1(8)
C(a3)–C(m1)–C(a2)	123.91(18)		
C(a3)–C(m1)–C(11)	118.42(18)		

^aThe estimated standard deviations of the least significant digits are given in parentheses.

Table S17. Anisotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.^a

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0154(1)	0.0143(1)	0.0221(1)	-0.0008(1)	0.0009(1)	-0.0017(1)
N(1)	0.0180(7)	0.0170(7)	0.0214(8)	-0.0019(7)	0.0026(6)	-0.0020(6)
N(2)	0.0192(8)	0.0174(7)	0.0268(9)	-0.0013(6)	0.0029(7)	-0.0016(6)
N(3)	0.0173(7)	0.0154(7)	0.0254(8)	-0.0006(7)	0.0006(6)	-0.0014(6)
N(4)	0.0173(7)	0.0166(7)	0.0231(8)	-0.0011(6)	0.0002(6)	-0.0010(6)
C(A1)	0.0173(8)	0.0213(9)	0.0205(9)	-0.0011(8)	0.0015(8)	-0.0020(7)
C(A2)	0.0188(8)	0.0196(9)	0.0195(9)	-0.0002(7)	0.0030(7)	-0.0001(7)
C(A3)	0.0214(9)	0.0187(9)	0.0266(10)	-0.0005(8)	0.0024(9)	0.0000(7)
C(A4)	0.0203(9)	0.0163(8)	0.0308(11)	-0.0010(8)	0.0014(8)	-0.0026(7)
C(A5)	0.0161(8)	0.0201(9)	0.0232(10)	0.0003(7)	0.0008(7)	-0.0023(7)
C(A6)	0.0169(9)	0.0182(9)	0.0260(10)	-0.0005(8)	-0.0007(7)	-0.0006(7)
C(A7)	0.0201(9)	0.0159(9)	0.0245(10)	0.0002(7)	0.0001(8)	0.0006(7)
C(A8)	0.0199(9)	0.0177(9)	0.0197(9)	-0.0010(7)	-0.0004(7)	-0.0032(7)
C(B1)	0.0176(9)	0.0241(9)	0.0260(10)	-0.0027(8)	0.0020(8)	-0.0018(7)
C(B2)	0.0179(9)	0.0240(9)	0.0247(10)	-0.0016(8)	0.0022(8)	0.0006(7)
C(B3)	0.0255(10)	0.0188(9)	0.0375(12)	-0.0048(9)	0.0041(9)	-0.0012(8)
C(B4)	0.0250(10)	0.0172(9)	0.0368(12)	-0.0037(9)	0.0031(9)	-0.0031(8)
C(B5)	0.0175(9)	0.0208(9)	0.0303(11)	0.0003(8)	0.0019(8)	-0.0026(7)
C(B6)	0.0174(9)	0.0199(9)	0.0315(11)	0.0007(8)	0.0010(8)	-0.0015(7)
C(B7)	0.0225(9)	0.0178(9)	0.0271(10)	-0.0003(8)	0.0003(8)	-0.0020(7)
C(B8)	0.0214(9)	0.0162(9)	0.0273(10)	0.0003(8)	-0.0007(8)	-0.0026(7)
C(M1)	0.0215(9)	0.0192(9)	0.0241(10)	-0.0023(8)	0.0030(8)	0.0010(7)
C(M2)	0.0198(9)	0.0176(9)	0.0265(10)	-0.0001(8)	0.0023(8)	-0.0038(7)
C(M3)	0.0205(9)	0.0157(9)	0.0282(10)	0.0019(8)	-0.0008(8)	0.0009(7)
C(M4)	0.0186(9)	0.0184(9)	0.0208(9)	0.0005(7)	-0.0007(7)	-0.0044(7)
C(11)	0.0170(9)	0.0178(9)	0.0292(10)	-0.0031(8)	0.0008(8)	-0.0012(7)
C(12)	0.0233(10)	0.0218(10)	0.0278(11)	0.0015(8)	0.0008(8)	0.0008(8)
C(13)	0.0216(10)	0.0261(10)	0.0315(11)	-0.0037(9)	0.0043(9)	0.0008(8)
C(14)	0.0168(9)	0.0220(10)	0.0421(13)	-0.0025(9)	0.0006(9)	0.0011(8)
C(15)	0.0241(10)	0.0261(10)	0.0388(13)	0.0051(9)	-0.0057(9)	0.0024(8)
C(16)	0.0249(10)	0.0292(11)	0.0272(10)	0.0007(9)	-0.0006(9)	0.0007(8)
C(21)	0.0186(9)	0.0157(8)	0.0310(12)	-0.0015(7)	0.0028(8)	-0.0021(7)
C(22)	0.0284(10)	0.0246(10)	0.0274(11)	-0.0017(9)	0.0012(8)	-0.0049(9)
C(23)	0.0284(11)	0.0233(10)	0.0370(13)	0.0022(9)	0.0086(10)	-0.0064(9)

Table S17. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	0.0200(9)	0.0174(9)	0.0453(13)	-0.0042(9)	0.0042(9)	-0.0048(7)
C(25)	0.0281(11)	0.0272(11)	0.0336(12)	-0.0057(9)	-0.0053(9)	-0.0033(9)
C(26)	0.0254(10)	0.0223(10)	0.0270(11)	0.0007(8)	0.0012(8)	-0.0041(8)
C(31)	0.0191(9)	0.0138(8)	0.0415(13)	0.0042(8)	0.0034(9)	0.0007(7)
C(32)	0.0258(11)	0.0213(10)	0.0418(13)	0.0033(9)	0.0087(9)	0.0008(8)
C(33)	0.0357(13)	0.0220(11)	0.0573(17)	-0.0016(11)	0.0185(12)	0.0017(10)
C(34)	0.0258(11)	0.0202(11)	0.079(2)	0.0034(12)	0.0151(13)	0.0026(9)
C(35)	0.0225(10)	0.0261(11)	0.075(2)	0.0094(13)	-0.0077(12)	0.0018(9)
C(36)	0.0240(10)	0.0224(10)	0.0541(15)	0.0010(11)	-0.0058(11)	-0.0001(8)
C(41)	0.0159(8)	0.0179(9)	0.0257(10)	-0.0001(7)	-0.0012(7)	-0.0008(7)
C(42)	0.0246(10)	0.0237(10)	0.0242(10)	0.0001(8)	0.0005(8)	-0.0040(8)
C(43)	0.0252(10)	0.0234(10)	0.0279(11)	-0.0026(8)	-0.0049(8)	-0.0042(8)
C(44)	0.0175(9)	0.0214(9)	0.0352(11)	0.0024(8)	-0.0033(9)	-0.0025(8)
C(45)	0.0191(9)	0.0239(10)	0.0294(11)	0.0024(9)	0.0028(8)	-0.0040(7)
C(46)	0.0208(9)	0.0216(9)	0.0243(10)	-0.0006(8)	-0.0002(8)	-0.0016(7)
N(5)	0.0230(9)	0.0191(8)	0.0245(8)	0.0000(7)	-0.0003(7)	-0.0060(6)
O(1)	0.0280(8)	0.0336(9)	0.0323(9)	0.0084(7)	-0.0063(7)	-0.0035(7)
N(6)	0.0219(8)	0.0182(8)	0.0247(9)	0.0001(7)	0.0035(7)	0.0036(6)
C(1)	0.0308(11)	0.0215(10)	0.0292(11)	0.0028(8)	0.0050(9)	0.0074(8)
C(2)	0.0302(11)	0.0243(10)	0.0313(11)	0.0015(9)	0.0000(9)	0.0074(9)
C(3)	0.0361(12)	0.0344(12)	0.0277(11)	-0.0005(9)	0.0050(10)	0.0134(10)
C(4)	0.0276(10)	0.0287(11)	0.0271(10)	0.0029(9)	0.0064(8)	0.0102(9)
N(7)	0.0502(13)	0.0410(12)	0.0376(12)	0.0061(10)	0.0066(10)	0.0089(10)
C(5)	0.0621(18)	0.0430(14)	0.0307(12)	0.0031(11)	0.0050(13)	0.0131(14)
Cl(1)	0.0388(5)	0.0438(5)	0.0502(6)	0.0053(5)	0.0129(4)	0.0173(4)
Cl(2)	0.0269(5)	0.0831(9)	0.0487(6)	-0.0175(6)	0.0040(4)	-0.0106(5)
Cl(3)	0.0476(7)	0.0813(12)	0.0661(9)	-0.0338(9)	-0.0039(7)	-0.0114(7)
C(6)	0.0249(17)	0.0283(17)	0.0372(19)	0.0127(15)	0.0113(14)	-0.0021(14)
Cl(1A)	0.0476(14)	0.0580(16)	0.182(5)	-0.030(3)	0.022(2)	-0.0168(12)
Cl(2A)	0.136(4)	0.087(2)	0.108(3)	-0.018(2)	0.037(3)	-0.054(3)
Cl(3A)	0.149(4)	0.090(3)	0.124(4)	0.052(3)	0.042(3)	0.032(3)
C(6A)	0.050(5)	0.026(4)	0.162(13)	0.040(6)	0.022(7)	0.022(4)

^aThe estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2 \pi [h^2 U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Table S18. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2) for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.^a

atom	x	y	z	U(eq)
H(B1)	0.6265	0.1283	0.7301	0.027
H(B2)	0.6332	0.2246	0.7789	0.027
H(B3)	0.8539	0.3646	0.8267	0.033
H(B4)	0.9937	0.3622	0.8004	0.032
H(B5)	1.1936	0.2158	0.6687	0.027
H(B6)	1.1884	0.1189	0.6230	0.027
H(B7)	0.9709	-0.0260	0.6406	0.027
H(B8)	0.8306	-0.0233	0.6624	0.026
H(12)	0.7103	0.2919	1.0176	0.029
H(13)	0.6184	0.3571	1.0618	0.032
H(14)	0.5783	0.4133	0.8905	0.032
H(15)	0.6275	0.4040	0.6735	0.036
H(16)	0.7182	0.3388	0.6296	0.033
H(22)	1.1281	0.3169	0.5452	0.032
H(23)	1.2262	0.3789	0.5633	0.035
H(24)	1.2735	0.4024	0.7735	0.033
H(25)	1.2252	0.3616	0.9672	0.036
H(26)	1.1260	0.3005	0.9488	0.030
H(32)	1.0638	0.0129	0.4301	0.036
H(33)	1.1561	-0.0520	0.3861	0.046
H(34)	1.2461	-0.0720	0.5468	0.050
H(35)	1.2455	-0.0296	0.7539	0.049
H(36)	1.1543	0.0359	0.7997	0.040
H(42)	0.7175	0.0220	0.4873	0.029
H(43)	0.6221	-0.0419	0.4743	0.031
H(44)	0.5542	-0.0658	0.6663	0.030
H(45)	0.5815	-0.0253	0.8725	0.029
H(46)	0.6748	0.0408	0.8845	0.027
H(1A)	0.9058	0.2681	0.5051	0.033
H(1B)	0.8202	0.2483	0.5214	0.033
H(2A)	0.8116	0.2313	0.2912	0.034
H(2B)	0.8379	0.2913	0.3130	0.034
H(3A)	0.9058	0.1622	0.2304	0.039
H(3B)	0.9931	0.1778	0.2106	0.039

Table S18. Continued

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
H(4A)	0.9743	0.1370	0.4218	0.033
H(4B)	1.0057	0.1959	0.4399	0.033
H(5A)	0.8735	0.2295	0.0565	0.068
H(5B)	0.9576	0.2528	0.0431	0.068
H(5C)	0.8888	0.2910	0.0830	0.068
H(6)	0.4143	0.1226	0.4588	0.036
H(6A)	0.5167	0.0550	0.6502	0.095

^a *U*(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor the estimated standard deviations of the least significant digits are given in parentheses.

Table S19. Complete Crystallographic Details for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl

formula	C ₇₅ H ₂₆₉ N ₁₀ O ₅ ClFe
FW, amu	1281.70
<i>a</i> , Å	18.6671(8)
<i>b</i> , Å	19.1581(8)
<i>c</i> , Å	18.4010(8)
β, deg	90.9050(10)
<i>V</i> , Å ³	6579.9(5)
space group	C2/c
<i>Z</i>	4
D _c , g/cm ³	1.294
F(000)	2688
μ, mm ⁻¹	0.330
crystal dimensions, mm	0.32 × 0.28 × 0.26
radiation	MoKα, λ = 0.71073 Å
temperature, K	100(2)
diffractometer	Enraf Nonius FAST
θ range for collected data, deg	2.13–28.30
index range	$-24 \leq h \leq 24$ $-25 \leq k \leq 25$ $-24 \leq l \leq 24$
total data collected	34949
absorption correction	Empirical
relative transmission coefficients (I)	1.000 and 0.8657
unique data	8181 ($R_{\text{int}} = 0.0294$)
unique observed data [$I > 2\sigma(I)$]	8181
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	R1 = 8181 / 0 / 421
goodness-of-fit (based on F^2)	R1 = 1.771
final <i>R</i> indices [$I > 2\sigma(I)$]	$R_1 = 0.1223$, $wR_2 = 0.3805$
final <i>R</i> indices (all data)	$R_1 = 0.1392$, $wR_2 = 0.4085$

Table S20. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2) for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl^a

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
Fe(1)	0.0000	0.35539(3)	0.7500	0.0284(3)
N(1)	0.04500(18)	0.36064(15)	0.84979(18)	0.0321(7)
N(2)	0.09759(18)	0.35881(15)	0.70584(18)	0.0327(7)
C(a1)	0.0104(2)	0.36471(19)	0.9147(2)	0.0355(8)
C(a2)	0.1163(2)	0.35710(17)	0.8668(2)	0.0335(8)
C(a3)	0.1624(2)	0.35450(18)	0.7418(2)	0.0338(8)
C(a4)	0.1132(2)	0.3606(2)	0.6327(2)	0.0365(8)
C(b1)	0.0618(2)	0.3640(2)	0.9742(2)	0.0413(9)
C(b2)	0.1273(2)	0.3602(2)	0.9447(2)	0.0402(9)
C(b3)	0.2200(2)	0.3535(2)	0.6912(2)	0.0406(9)
C(b4)	0.1897(2)	0.3567(2)	0.6233(2)	0.0432(10)
C(m1)	0.0643(2)	0.3657(2)	0.5762(2)	0.0385(8)
C(m2)	0.1724(2)	0.35465(17)	0.8170(2)	0.0329(8)
C(1)	0.0917(2)	0.3730(2)	0.5008(2)	0.0424(9)
C(2)	0.0946(3)	0.4398(3)	0.4688(3)	0.0560(12)
C(3)	0.1213(3)	0.4487(3)	0.3994(3)	0.0615(14)
C(4)	0.1458(2)	0.3914(4)	0.3621(3)	0.0679(18)
C(5)	0.1424(2)	0.3237(3)	0.3923(2)	0.0536(12)
C(6)	0.1152(2)	0.3158(2)	0.4609(2)	0.0445(10)
N(3)	0.1116(3)	0.2491(2)	0.4958(2)	0.0708(15)
C(7)	0.1247(9)	0.1867(8)	0.4822(8)	0.238(11)
O(1)	0.1306(5)	0.1649(4)	0.4114(4)	0.136(2)
C(8)	0.1112(5)	0.1315(4)	0.5390(4)	0.088(2)
C(9a)	0.1789(5)	0.1037(6)	0.5448(6)	0.063(2)
C(10a)	0.0533(4)	0.0726(5)	0.5141(7)	0.076(3)
C(11a)	0.0843(9)	0.1532(6)	0.6153(8)	0.100(5)
C(9b)	0.1809(8)	0.0788(8)	0.5188(9)	0.060(4)
C(10b)	0.0561(13)	0.1207(13)	0.5399(13)	0.093(5)
C(11b)	0.1430(15)	0.1688(14)	0.6301(14)	0.111(7)
C(12)	0.2478(2)	0.35407(19)	0.8456(2)	0.0367(8)
C(13)	0.2874(2)	0.4164(2)	0.8455(2)	0.0436(9)
C(14)	0.3585(3)	0.4175(3)	0.8697(3)	0.0550(12)
C(15)	0.3888(3)	0.3571(3)	0.8964(3)	0.0639(16)
C(16)	0.3515(2)	0.2957(3)	0.8976(3)	0.0643(15)

Table S20. Continued

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
C(17)	0.2804(2)	0.2931(2)	0.8716(3)	0.0441(9)
N(4)	0.23974(18)	0.2308(2)	0.8707(3)	0.0585(12)
C(18)	0.2625(2)	0.1650(2)	0.8737(2)	0.0461(10)
O(2)	0.3236(2)	0.1494(2)	0.8858(3)	0.0743(13)
C(19)	0.2052(3)	0.1079(3)	0.8644(3)	0.0605(13)
C(20)	0.1366(6)	0.1256(7)	0.8842(9)	0.212(9)
C(21)	0.2152(7)	0.0721(8)	0.7994(7)	0.227(10)
C(22)	0.2221(11)	0.0523(8)	0.9248(14)	0.320(16)
N(5)	0.0000	0.2644(2)	0.7500	0.0355(9)
O(3)	0.0351(6)	0.2216(5)	0.7815(6)	0.202(5)
N(6)	0.0000	0.4734(2)	0.7500	0.0385(10)
C(23)	-0.0413(2)	0.5093(2)	0.7953(3)	0.0487(11)
C(24)	-0.0424(3)	0.5815(3)	0.7970(4)	0.0711(18)
C(25)	0.0000	0.61896(12)	0.7500	0.071(3)
Cl(1)	0.0000	0.02499(12)	0.7500	0.1280(14)
C(26)	-0.0110	-0.06164(12)	0.7389	0.052(2)
C(27)	-0.0560	-0.07837(12)	0.6950	0.062(3)
C(28)	-0.0730	-0.14599(12)	0.6750	0.067(3)
C(29)	-0.0232	-0.19208(12)	0.7030	0.124(7)
C(30)	0.0279	-0.17289(12)	0.7590	0.111(6)
C(31)	0.0320	-0.11937(12)	0.7760	0.060(2)

^a *U*(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S21. Bond Lengths for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl^a

bond	length (Å)	bond	length (Å)
Fe(1)–N(5)	1.742(5)	C(16)–C(17)	1.405(6)
Fe(1)–N(2)	2.007(3)	C(17)–N(4)	1.414(6)
Fe(1)–N(2)#1	2.007(3)	N(4)–C(18)	1.332(6)
Fe(1)–N(1)	2.010(3)	C(18)–O(2)	1.196(6)
Fe(1)–N(1)#1	2.010(3)	C(18)–C(19)	1.539(7)
Fe(1)–N(6)	2.260(5)	C(19)–C(20)	1.379(11)
N(1)–C(a2)	1.364(5)	C(19)–C(21)	1.393(10)
N(1)–C(a1)	1.369(5)	C(19)–C(22)	1.568(15)
N(2)–C(a3)	1.373(5)	N(5)–O(3)	1.194(9)
N(2)–C(a4)	1.382(5)	N(5)–O(3)#1	1.194(9)
C(a1)–C(m1#1)	1.407(6)	O(3)–O(3)#1	1.74(2)
C(a1)–C(b1)	1.445(5)	N(6)–C(23)#1	1.335(5)
C(a2)–C(m2)	1.402(6)	N(6)–C(23)	1.335(5)
C(a2)–C(b2)	1.447(5)	C(23)–C(24)	1.384(6)
C(a3)–C(m2)	1.394(6)	C(24)–C(25)	1.382(8)
C(a3)–C(b3)	1.434(6)	C(25)–C(24)#1	1.382(8)
C(a4)–C(m1)	1.377(6)	Cl(1)–C(26)#1	1.6843
C(a4)–C(b4)	1.442(6)	Cl(1)–C(26)	1.6844
C(b1)–C(b2)	1.347(6)	C(26)–C(26)#1	0.5747
C(b3)–C(b4)	1.365(6)	C(26)–C(27)	1.1998
C(m1)–C(a1#1)	1.407(6)	C(26)–C(31)#1	1.2036
C(m1)–C(1)	1.493(6)	C(26)–C(31)	1.5219
C(m2)–C(12)	1.495(5)	C(26)–C(27)#1	1.7602
C(1)–C(6)	1.394(7)	C(27)–C(31)#1	1.0464
C(1)–C(2)	1.408(6)	C(27)–C(28)	1.3822
C(2)–C(3)	1.389(7)	C(27)–C(26)#1	1.7602
C(3)–C(4)	1.377(9)	C(28)–C(31)#1	1.2794
C(4)–C(5)	1.413(8)	C(28)–C(29)	1.3763
C(5)–C(6)	1.376(6)	C(28)–C(30)#1	1.5546
C(6)–N(3)	1.433(6)	C(29)–C(30)#1	0.7961
N(3)–C(7)	1.246(15)	C(29)–C(30)	1.4408
C(7)–O(1)	1.375(17)	C(29)–C(31)#1	1.4555
C(7)–C(8)	1.511(11)	C(29)–C(29)#1	1.9221
C(8)–C(10b)	1.05(2)	C(30)–C(29)#1	0.7961

Table S21. Continued

bond	length (Å)	bond	length (Å)
C(8)–C(9a)	1.375(12)	C(30)–C(31)	1.0743
C(8)–C(11a)	1.555(16)	C(30)–C(30)#1	1.0881
C(8)–C(10a)	1.624(12)	C(30)–C(28)#1	1.5546
C(8)–C(9b)	1.694(17)	C(30)–C(31)#1	1.6412
C(8)–C(11b)	1.91(3)	C(31)–C(27)#1	1.0464
C(12)–C(17)	1.399(6)	C(31)–C(26)#1	1.2037
C(12)–C(13)	1.404(5)	C(31)–C(28)#1	1.2793
C(13)–C(14)	1.393(6)	C(31)–C(29)#1	1.4555
C(14)–C(15)	1.377(8)	C(31)–C(31)#1	1.5188
C(15)–C(16)	1.366(7)	C(31)–C(30)#1	1.6412

^aThe estimated standard deviations of the least significant digits are given in parentheses.

Table S22. Bond Angles for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl^a

angle	degree	angle	degree
N(5)–Fe(1)–N(2)	91.87(8)	C(20)–C(19)–C(22)	99.0(13)
N(5)–Fe(1)–N(2)#1	91.87(8)	C(21)–C(19)–C(22)	104.2(13)
N(2)–Fe(1)–N(2)#1	176.26(16)	C(18)–C(19)–C(22)	105.7(6)
N(5)–Fe(1)–N(1)	92.87(8)	O(3)–N(5)–O(3)#1	93.3(10)
N(2)–Fe(1)–N(1)	89.96(14)	O(3)–N(5)–Fe(1)	133.4(5)
N(2)#1–Fe(1)–N(1)	89.85(14)	O(3)#1–N(5)–Fe(1)	133.4(5)
N(5)–Fe(1)–N(1)#1	92.86(8)	N(5)–O(3)–O(3)#1	43.4(5)
N(2)–Fe(1)–N(1)#1	89.85(14)	C(23)#1–N(6)–C(23)	118.0(6)
N(2)#1–Fe(1)–N(1)#1	89.96(14)	C(23)#1–N(6)–Fe(1)	121.0(3)
N(1)–Fe(1)–N(1)#1	174.27(16)	C(23)–N(6)–Fe(1)	121.0(3)
N(5)–Fe(1)–N(6)	180.000(1)	N(6)–C(23)–C(24)	122.6(6)
N(2)–Fe(1)–N(6)	88.13(8)	C(25)–C(24)–C(23)	119.7(5)
N(2)#1–Fe(1)–N(6)	88.13(8)	C(24)#1–C(25)–C(24)	117.4(5)
N(1)–Fe(1)–N(6)	87.13(8)	C(26)#1–Cl(1)–C(26)	19.6
N(1)#1–Fe(1)–N(6)	87.14(8)	C(26)#1–C(26)–C(27)	164.5
C(a2)–N(1)–C(a1)	106.0(3)	C(26)#1–C(26)–C(31)#1	112.9
C(a2)–N(1)–Fe(1)	126.8(3)	C(27)–C(26)–C(31)#1	51.6
C(a1)–N(1)–Fe(1)	127.1(3)	C(26)#1–C(26)–C(31)	46.8
C(a3)–N(2)–C(a4)	105.8(3)	C(27)–C(26)–C(31)	117.8
C(a3)–N(2)–Fe(1)	127.0(3)	C(31)#1–C(26)–C(31)	66.5
C(a4)–N(2)–Fe(1)	127.0(3)	C(26)#1–C(26)–Cl(1)	80.2
N(1)–C(a1)–C(m1)#1	125.9(4)	C(27)–C(26)–Cl(1)	115.3
N(1)–C(a1)–C(b1)	110.1(4)	C(31)#1–C(26)–Cl(1)	166.3
C(m1)#1–C(a1)–C(b1)	123.9(4)	C(31)–C(26)–Cl(1)	126.8
N(1)–C(a2)–C(m2)	126.0(4)	C(26)#1–C(26)–C(27)#1	10.5
N(1)–C(a2)–C(b2)	110.3(4)	C(27)–C(26)–C(27)#1	154.0
C(m2)–C(a2)–C(b2)	123.6(4)	C(31)#1–C(26)–C(27)#1	102.4
N(2)–C(a3)–C(m2)	125.5(4)	C(31)–C(26)–C(27)#1	36.3
N(2)–C(a3)–C(b3)	110.6(4)	Cl(1)–C(26)–C(27)#1	90.7
C(m2)–C(a3)–C(b3)	123.8(4)	C(31)#1–C(27)–C(26)	64.4
C(m1)–C(a4)–N(2)	126.1(4)	C(31)#1–C(27)–C(28)	61.8
C(m1)–C(a4)–C(b4)	124.0(4)	C(26)–C(27)–C(28)	125.8
N(2)–C(a4)–C(b4)	109.9(4)	C(31)#1–C(27)–C(26)#1	59.4
C(b2)–C(b1)–C(a1)	106.9(4)	C(26)–C(27)–C(26)#1	5.0

Table S22. Continued

angle	degree	angle	degree
C(b1)–C(b2)–C(a2)	106.7(4)	C(28)–C(27)–C(26)#1	120.8
C(b4)–C(b3)–C(a3)	106.8(4)	C(31)#1–C(28)–C(29)	66.4
C(b3)–C(b4)–C(a4)	106.8(4)	C(31)#1–C(28)–C(27)	46.1
C(a4)–C(m1)–C(a1#1)	123.8(4)	C(29)–C(28)–C(27)	110.5
C(a4)–C(m1)–C(1)	118.4(4)	C(31)#1–C(28)–C(30)#1	43.2
C(a1#1)–C(m1)–C(1)	117.9(4)	C(29)–C(28)–C(30)#1	30.8
C(a3)–C(m2)–C(a2)	124.1(4)	C(27)–C(28)–C(30)#1	89.1
C(a3)–C(m2)–C(12)	117.3(4)	C(30)#1–C(29)–C(28)	87.1
C(a2)–C(m2)–C(12)	118.6(4)	C(30)#1–C(29)–C(30)	48.3
C(6)–C(1)–C(2)	118.6(4)	C(28)–C(29)–C(30)	122.7
C(6)–C(1)–C(m1)	122.1(4)	C(30)#1–C(29)–C(31)#1	46.4
C(2)–C(1)–C(m1)	119.3(4)	C(28)–C(29)–C(31)#1	53.6
C(3)–C(2)–C(1)	120.8(5)	C(30)–C(29)–C(31)#1	69.0
C(4)–C(3)–C(2)	119.1(5)	C(30)#1–C(29)–C(29)#1	42.6
C(3)–C(4)–C(5)	121.2(5)	C(28)–C(29)–C(29)#1	129.0
C(6)–C(5)–C(4)	118.7(6)	C(30)–C(29)–C(29)#1	22.0
C(5)–C(6)–C(1)	121.4(4)	C(31)#1–C(29)–C(29)#1	79.2
C(5)–C(6)–N(3)	122.0(5)	C(29)#1–C(30)–C(31)	101.1
C(1)–C(6)–N(3)	116.6(4)	C(29)#1–C(30)–C(30)#1	98.6
C(7)–N(3)–C(6)	139.1(6)	C(31)–C(30)–C(30)#1	98.7
N(3)–C(7)–O(1)	120.1(7)	C(29)#1–C(30)–C(29)	115.4
N(3)–C(7)–C(8)	119.9(9)	C(31)–C(30)–C(29)	119.7
O(1)–C(7)–C(8)	117.3(14)	C(30)#1–C(30)–C(29)	33.1
C(10b)–C(8)–C(9a)	145.4(16)	C(29)#1–C(30)–C(28)#1	62.2
C(10b)–C(8)–C(7)	108.8(16)	C(31)–C(30)–C(28)#1	54.6
C(9a)–C(8)–C(7)	99.3(8)	C(30)#1–C(30)–C(28)#1	137.9
C(10b)–C(8)–C(11a)	73.0(16)	C(29)–C(30)–C(28)#1	170.9
C(9a)–C(8)–C(11a)	110.2(9)	C(29)#1–C(30)–C(31)#1	123.3
C(7)–C(8)–C(11a)	119.8(9)	C(31)–C(30)–C(31)#1	64.1
C(10b)–C(8)–C(10a)	38.7(14)	C(30)#1–C(30)–C(31)#1	40.3
C(9a)–C(8)–C(10a)	111.1(8)	C(29)–C(30)–C(31)#1	55.9
C(7)–C(8)–C(10a)	114.1(11)	C(28)#1–C(30)–C(31)#1	117.2
C(11a)–C(8)–C(10a)	102.6(9)	C(27)#1–C(31)–C(30)	153.2
C(10b)–C(8)–C(9b)	130.0(17)	C(27)#1–C(31)–C(26)#1	64.0

Table S22. Continued

angle	degree	angle	degree
C(9a)–C(8)–C(9b)	22.5(6)	C(30)–C(31)–C(26)#1	142.1
C(7)–C(8)–C(9b)	97.4(8)	C(27)#1–C(31)–C(28)#1	72.1
C(11a)–C(8)–C(9b)	128.2(9)	C(30)–C(31)–C(28)#1	82.2
C(10a)–C(8)–C(9b)	92.0(8)	C(26)#1–C(31)–C(28)#1	135.7
C(10b)–C(8)–C(11b)	110.6(18)	C(27)#1–C(31)–C(29)#1	129.2
C(9a)–C(8)–C(11b)	78.7(10)	C(30)–C(31)–C(29)#1	32.5
C(7)–C(8)–C(11b)	107.0(13)	C(26)#1–C(31)–C(29)#1	154.4
C(11a)–C(8)–C(11b)	37.6(9)	C(28)#1–C(31)–C(29)#1	60.0
C(10a)–C(8)–C(11b)	134.8(11)	C(27)#1–C(31)–C(31)#1	130.3
C(9b)–C(8)–C(11b)	100.7(11)	C(30)–C(31)–C(31)#1	76.4
C(17)–C(12)–C(13)	118.9(4)	C(26)#1–C(31)–C(31)#1	66.8
C(17)–C(12)–C(m2)	122.0(3)	C(28)#1–C(31)–C(31)#1	154.1
C(13)–C(12)–C(m2)	119.1(4)	C(29)#1–C(31)–C(31)#1	94.4
C(14)–C(13)–C(12)	120.8(4)	C(27)#1–C(31)–C(26)	84.4
C(15)–C(14)–C(13)	119.0(4)	C(30)–C(31)–C(26)	121.9
C(16)–C(15)–C(14)	121.5(5)	C(26)#1–C(31)–C(26)	20.4
C(15)–C(16)–C(17)	120.3(5)	C(28)#1–C(31)–C(26)	155.7
C(12)–C(17)–C(16)	119.4(4)	C(29)#1–C(31)–C(26)	138.9
C(12)–C(17)–N(4)	118.0(3)	C(31)#1–C(31)–C(26)	46.6
C(16)–C(17)–N(4)	122.6(4)	C(27)#1–C(31)–C(30)#1	162.3
C(18)–N(4)–C(17)	128.8(4)	C(30)–C(31)–C(30)#1	40.9
O(2)–C(18)–N(4)	123.2(5)	C(26)#1–C(31)–C(30)#1	105.5
O(2)–C(18)–C(19)	120.2(5)	C(28)#1–C(31)–C(30)#1	115.1
N(4)–C(18)–C(19)	116.6(4)	C(29)#1–C(31)–C(30)#1	55.1
C(20)–C(19)–C(21)	119.0(9)	C(31)#1–C(31)–C(30)#1	39.5
C(20)–C(19)–C(18)	116.3(5)	C(26)–C(31)–C(30)#1	85.8
C(21)–C(19)–C(18)	110.1(5)		

^aThe estimated standard deviations of the least significant digits are given in parentheses.

Table S23. Anisotropic Displacement Parameters (\AA^2) for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl^a

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0288(4)	0.0265(4)	0.0296(4)	0.000	-0.0064(3)	0.000
N(1)	0.0313(15)	0.0317(15)	0.0329(15)	-0.0042(11)	-0.0056(12)	0.0043(11)
N(2)	0.0341(16)	0.0340(16)	0.0298(15)	-0.0004(11)	-0.0066(12)	0.0016(11)
C(a1)	0.0375(19)	0.0346(18)	0.0340(19)	-0.0072(14)	-0.0092(15)	0.0050(14)
C(a2)	0.0361(19)	0.0302(17)	0.0339(18)	-0.0064(13)	-0.0096(15)	0.0059(13)
C(a3)	0.0300(18)	0.0342(18)	0.0369(19)	-0.0001(13)	-0.0046(14)	0.0013(13)
C(a4)	0.0337(19)	0.042(2)	0.0331(19)	0.0035(14)	-0.0043(15)	-0.0024(14)
C(b1)	0.042(2)	0.050(2)	0.0311(18)	-0.0077(15)	-0.0104(16)	0.0028(17)
C(b2)	0.038(2)	0.048(2)	0.035(2)	-0.0085(15)	-0.0117(16)	0.0062(15)
C(b3)	0.034(2)	0.051(2)	0.036(2)	-0.0016(16)	-0.0064(16)	0.0014(15)
C(b4)	0.036(2)	0.059(3)	0.034(2)	0.0011(16)	-0.0018(16)	0.0005(17)
C(m1)	0.038(2)	0.044(2)	0.0340(19)	0.0035(15)	-0.0050(15)	-0.0030(15)
C(m2)	0.0332(19)	0.0286(17)	0.0366(19)	-0.0024(12)	-0.0087(14)	0.0012(12)
C(1)	0.0353(19)	0.055(2)	0.036(2)	0.0121(17)	-0.0070(15)	-0.0108(17)
C(2)	0.058(3)	0.059(3)	0.050(3)	0.021(2)	-0.010(2)	-0.006(2)
C(3)	0.063(3)	0.069(3)	0.052(3)	0.033(2)	-0.010(2)	-0.013(3)
C(4)	0.034(2)	0.123(5)	0.046(3)	0.041(3)	-0.0078(19)	-0.018(3)
C(5)	0.040(2)	0.088(4)	0.033(2)	0.015(2)	-0.0047(16)	-0.002(2)
C(6)	0.043(2)	0.057(3)	0.0329(19)	0.0073(17)	-0.0026(16)	-0.0117(18)
N(3)	0.126(5)	0.051(2)	0.035(2)	-0.0046(17)	0.009(2)	-0.014(3)
C(7)	0.276(16)	0.246(14)	0.196(12)	0.171(12)	0.194(13)	0.207(13)
O(1)	0.168(7)	0.129(5)	0.111(5)	-0.004(4)	0.027(5)	0.041(5)
C(8)	0.087(5)	0.088(5)	0.088(5)	0.045(4)	-0.008(4)	0.012(4)
C(9a)	0.042(4)	0.068(6)	0.079(6)	-0.014(5)	-0.002(4)	-0.010(4)
C(10a)	0.040(4)	0.069(6)	0.118(8)	0.042(6)	-0.042(5)	-0.020(4)
C(11a)	0.119(11)	0.075(7)	0.107(10)	0.045(7)	0.031(9)	0.007(7)
C(12)	0.0328(19)	0.041(2)	0.0364(19)	-0.0033(14)	-0.0037(15)	-0.0018(14)
C(13)	0.048(2)	0.040(2)	0.043(2)	-0.0060(16)	-0.0015(17)	-0.0071(17)
C(14)	0.050(3)	0.067(3)	0.048(2)	-0.014(2)	0.000(2)	-0.023(2)
C(15)	0.038(2)	0.095(4)	0.059(3)	0.006(3)	-0.017(2)	-0.020(2)
C(16)	0.035(2)	0.078(3)	0.079(4)	0.034(3)	-0.019(2)	-0.008(2)
C(17)	0.0325(19)	0.047(2)	0.053(2)	0.0080(18)	-0.0126(16)	-0.0040(16)
N(4)	0.0255(16)	0.043(2)	0.106(4)	0.015(2)	-0.0106(18)	0.0016(14)
C(18)	0.049(2)	0.046(2)	0.043(2)	0.0027(18)	-0.0017(18)	0.0087(19)

Table S23. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O(2)	0.063(2)	0.064(2)	0.095(3)	-0.0253(19)	-0.036(2)	0.0277(18)
C(19)	0.071(3)	0.043(2)	0.068(3)	0.002(2)	-0.003(3)	-0.005(2)
C(20)	0.127(8)	0.183(10)	0.330(19)	-0.176(12)	0.160(11)	-0.113(8)
C(21)	0.180(11)	0.318(18)	0.188(11)	-0.189(13)	0.128(10)	-0.192(13)
C(22)	0.31(2)	0.152(12)	0.49(4)	0.193(18)	-0.24(2)	-0.159(14)
N(5)	0.035(2)	0.032(2)	0.040(2)	0.000	-0.0036(18)	0.000
O(3)	0.253(12)	0.120(6)	0.230(11)	0.044(7)	-0.069(8)	-0.004(7)
N(6)	0.033(2)	0.032(2)	0.050(3)	0.000	-0.0148(19)	0.000
C(23)	0.044(2)	0.036(2)	0.065(3)	-0.0111(19)	-0.023(2)	0.0064(17)
C(24)	0.067(3)	0.042(3)	0.102(4)	-0.028(3)	-0.046(3)	0.015(2)
C(25)	0.068(5)	0.029(3)	0.115(7)	0.000	-0.046(5)	0.000
Cl(1)	0.112(2)	0.0586(14)	0.214(4)	0.000	0.021(2)	0.000

^aThe estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2 \pi [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Table S24. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (\AA^2) for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl^a

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
H(b1)	0.0515	0.3658	1.0246	0.050
H(b2)	0.1720	0.3597	0.9701	0.048
H(b3)	0.2698	0.3510	0.7026	0.049
H(b4)	0.2142	0.3565	0.5784	0.052
H(2)	0.0782	0.4791	0.4951	0.067
H(3)	0.1226	0.4938	0.3780	0.074
H(4)	0.1654	0.3975	0.3152	0.082
H(5)	0.1586	0.2844	0.3657	0.064
H(3a)	0.0951	0.2535	0.5401	0.085
H(9a1)	0.1765	0.0576	0.5677	0.095
H(9a2)	0.2094	0.1345	0.5744	0.095
H(9a3)	0.1992	0.0990	0.4962	0.095
H(10a)	0.0450	0.0405	0.5545	0.114
H(10b)	0.0717	0.0466	0.4725	0.114
H(10c)	0.0080	0.0953	0.5001	0.114
H(11a)	0.0361	0.1732	0.6105	0.150
H(11b)	0.1169	0.1881	0.6364	0.150
H(11c)	0.0829	0.1121	0.6470	0.150
H(9b1)	0.1725	0.0321	0.5387	0.089
H(9b2)	0.2252	0.0980	0.5401	0.089
H(9b3)	0.1856	0.0758	0.4659	0.089
H(10d)	0.0413	0.0993	0.4937	0.140
H(10e)	0.0295	0.1643	0.5469	0.140
H(10f)	0.0461	0.0886	0.5799	0.140
H(11d)	0.1050	0.1975	0.6508	0.166
H(11e)	0.1857	0.1975	0.6229	0.166
H(11f)	0.1546	0.1304	0.6635	0.166
H(13)	0.2655	0.4582	0.8287	0.052
H(14)	0.3856	0.4594	0.8678	0.066
H(15)	0.4368	0.3580	0.9144	0.077
H(16)	0.3738	0.2547	0.9161	0.077
H(4a)	0.1930	0.2363	0.8677	0.070
H(20a)	0.1387	0.1551	0.9276	0.318
H(20b)	0.1094	0.0831	0.8946	0.318

Table S24. Continued

atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> (eq)
H(20c)	0.1130	0.1511	0.8443	0.318
H(21a)	0.1836	0.0312	0.7976	0.341
H(21b)	0.2652	0.0568	0.7966	0.341
H(21c)	0.2038	0.1030	0.7584	0.341
H(22a)	0.1777	0.0391	0.9489	0.479
H(22b)	0.2558	0.0721	0.9606	0.479
H(22c)	0.2435	0.0108	0.9026	0.479
H(23)	-0.0711	0.4843	0.8276	0.058
H(24)	-0.0722	0.6052	0.8303	0.085
H(25)	0.0000	0.6685	0.7500	0.085

^a *U*(eq) is defined as one third of the trace of the orthogonalized \mathbf{U}_{ij} tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Supporting Information

Table S1. Complete Crystallographic Details for [Fe(TPP)(NO)(4-NMe₂Py)].

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for [Fe(TPP)(NO)(4-NMe₂Py)].

Table S3. Bond Lengths for [Fe(TPP)(NO)(4-NMe₂Py)].

Table S4. Bond Angles for [Fe(TPP)(NO)(4-NMe₂Py)].

Table S5. Anisotropic Isotropic Displacement Parameters for [Fe(TPP)(NO)(4-NMe₂Py)].

Table S6. Hydrogen Coordinates and Isotropic Displacement Parameters for [Fe(TPP)(NO)(4-NMe₂Py)].

Table S7. Complete Crystallographic Details for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.

Table S8. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.

Table S9. Bond Lengths for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.

Table S10. Bond Angles for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.

Table S11. Anisotropic Isotropic Displacement Parameters for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.

Table S12. Hydrogen Coordinates and Isotropic Displacement Parameters for [Fe(TPP)(NO)(1-MeIm)]·CHCl₃.

Table S13. Complete Crystallographic Details for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.

Table S14. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.

Table S15. Bond Lengths for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.

Table S16. Bond Angles for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.

Table S17. Anisotropic Isotropic Displacement Parameters for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.

Table S18. Hydrogen Coordinates and Isotropic Displacement Parameters for [Fe(TPP)(NO)(4-MePip)]·CHCl₃.

Table S19. Complete Crystallographic Details for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl.

Table S20. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl.

Table S21. Bond Lengths for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl.

Table S22. Bond Angles for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl.

Table S23. Anisotropic Displacement Parameters for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl.

Table S24. Hydrogen Coordinates and Isotropic Displacement Parameters for [Fe(TpivPP)(NO)(Py)]·C₆H₅Cl.